学位論文

Mesoscopic Thermodynamics based on Quantum Information Theory

（量子情報理論に基づくメゾスコピック系の熱力学）

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Abstract

The current research situation surrounding the small-size heat engines looks almost exactly like the one in 1700s surrounding the macroscopic heat engines, on the night before the appearance of thermodynamics. The development of experimental techniques is realizing micro-machines in laboratories, and is clarifying the functions of bio-moleculars which are micro-machines in nature. The development of theoretic analysis is also achieving a splendid success both in the microscopic and macroscopic limits. However, no theoretical study has sufficiently discussed thermodynamic laws in mesoscopic scales, where the number of particles is not so small but finite. There is also a problem in the formulation of quantum heat engines themselves; there are various formulations, but the relation among them has not been clarified.

The present thesis is devoted to reconsider the above two problems, using the quantum information theory. First, we reconsider the formulation for quantum heat engines by using quantum measurement theory. We give a trade-off inequality which means that we have to destroy the coherence of the thermodynamic system in order to know the amount of the extracted energy; namely, a work extraction must be a measurement. Based on the fact, we formulate the work extraction as a measurement process, and clarify the previous formulations in our framework.

Second, we assess how accurately thermodynamics gives an approximation to the optimal efficiency of heat engines composed of a finite-particle working body and finite-particle heat baths, by using large deviation theory. We microscopically derive a thermodynamical upper bound for the efficiency of finite-size heat engines with two heat baths that are composed of n identical particles. It is not the upper limit, but we can obtain an asymptotic approximation of the upper limit by expanding our upper bound asymptotically in terms of $q_n := Q_{H,n}/n$, where $Q_{H,n}$ is the extracted heat from the hot bath. In the case that the heat baths' particle are uncorrelated each others, the asymptotic expansion of our upper bound approximates the optimal efficiency up to the first order of q_n in general, and up to the second order of q_n^2 in the case that $Q_{H,n}$ is non-decreasing of n; there exists a thermodynamic operation whose asymptotic expansion of efficiency coincides with that of our upper bound up to the orders.

Publication List

Journal Articles

(i) H. Tajima, "Deterministic LOCC transformation for three qubit pure states," *Annals of Physics*, **329**, 1-27, (2013). (contains results presented in Appendix B)

(ii) H. Tajima, "Second law of information thermodynamics with entanglement transfer," *Physical Review E*, **88**, 042143 (2013). (contains results presented in Chapter 2)

Proceedings

(iii) H. Tajima, "A New Second Law of Information Thermodynamics Using Entanglement Measure," *JPS Conference Proceedings*, **1**, 012129 (2014). (contains results presented in Chapter 2)

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(iv) H. Tajima, "Minimal energy cost of thermodynamic information processes only with entanglement transfer," arXiv:1311.1285, (2013). (contains results presented in Chapter 2)

(v) H. Tajima and M. Hayashi, "Refined Carnot 's Thereom; Asymptotics of Thermodynamics with Finite-Size Heat Baths," arXiv:1405.6457, (2014). (contains results presented in Chapter 4)

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(vi) H. Tajima and M. Hayashi, "Work extraction as a measurement process." (contains results presented in Chapter 3)

Contents

Chapter 1

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. Probing and manipulating small-size systems has become possible, and now we are able to verify thermodynamic features of microscopic and mesoscopic systems [4–6].

However, there is no guarantee that we can apply the standard thermodynamics to the small-size heat engines as it is, because it is a phenomenology for macroscopic systems. The 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 [7–37]. The statistical mechanical approach has achieved splendid success in the following three topics;

statistic derivation of thermodynamical inequalities [7–12]

There are many results according to the statistic derivation of thermodynamic inequalities in classical and quantum systems. For quantum heat engines, Tasaki [8] has derived the principle of maximum work statistically. While he did not show the existence of the optimal operation which achieves the equality of the principle of maximum work. In 2014, Skrzypczyk, Short, and Popescu [12] showed the the principle of maximum work including its achievability in another setup.

Thermodynamic laws for processes with measurement and feedback [13–31]

When we perform measurement and feedback on a thermodynamical system, the second law of thermodynamics appears to be violated. This well-known fact was pointed out by Maxwell [13], and numerous studies have long been conducted on it [14–31]. Szilard [14] has pointed out that the violation is related to the information content, and Sagawa and Ueda [25] gave an upper bound of the extracted work by a thermodynamic process with measurement and feedback by generalizing Szilard's idea. Sagawa and Ueda [15] also gave a lower bound of the energy cost of the measurement and information erase process, by generalizing Landauer's principle.

Thermodynamic laws for the nano scale working bodies [32–37]

Many researches recently reported how the finiteness of the working body affects the thermodynamic laws for microscopic systems by statistical mechanical methods [32–37]. The key concept in Refs. [33–36] is the smooth entropy [43, 44], which is an extension of the Shannon entropy, and that in Ref. [37] is the entanglement catalyst theory [45], which is an important result in quantum information theory. In these results, the extractable amount of work by single-shot extraction from a microscopic system connected to a heat bath was given as a function of the failure probability [33, 35, 36] and criteria for "thermodynamic state transitions" were given [33, 37]. When the initial state of the system is $\rho^{\otimes n}$, that is when the system is composed of uncorrelated identical particles, these results reduce to the principle of maximum work in the limit $n \to \infty$.

However, in spite of these important progresses, the following two theoretical problems remain in the statistical mechanical approach.

- There is no quantitative understanding of thermodynamic laws for the systems whose number of particle is not so small but finite. In other words, we do not know thermodynamic laws in mesoscopic realms. The smooth entropy is a very general tool, but it is very difficult to compute, and thus it gives only formal solutions in such cases.

- The concept of the work extraction from the quantum systems is very subtle, and no consensus has been reached [38]. The previous researches on quantum systems [8–12, 25–31, 33–37] have been formulated in various ways, and the relationship among the formulations has not been sufficiently discussed. The formulations are roughly classified in the semi-classical scenario [8–10, 25–30] and the fully quantum scenario [11, 12, 31, 33–37]. In the semi-classical scenario, the heat engine and the heat baths evolutes 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 main theme of the present thesis is to revisit the above two problems and to give a useful method to analyze the thermodynamical features of the mesoscopic systems, based on the quantum information theory. First, we reconsider the formulation for quantum heat engines by using quantum measurement theory [41, 42] and show that there is a serious conflict between the semi-classical scenario and the fully quantum scenario. To be specific, as soon as we request the condition that we can know the amount of the extracted work by observing the work storage, we become unable to describe the time evolution as a unitary time evolution. This fact is given as a trade-off inequality which means that we have to destroy the coherence of the thermodynamic system in order to know the amount of the extracted energy; namely, a work extraction must be a measurement. Based on the fact, we give a several classes of the energy transfer from the internal system to the external system, whose elements satisfies the features which a work extraction should satisfy.

Second, we give a quantitative method to calculate the efficiency for heat engines in mesoscopic scales, and assess how accurately thermodynamics gives an approximation to the optimal efficiency. In order to overcome the problem of finitely large values of the particle number n, we need more detailed analytical tools than the smooth entropy; namely, the information geometry [59] and the strong large deviation theory [46, 47]. Using the information geometry, we microscopically rederive a thermodynamical upper bound for the efficiency of finite-size heat engines with two heat baths that are composed of n identical particles. Next, we asymptotically expand the upper bound in terms of $q_n := Q_{H,n}/n$, where the $Q_{H,n}$ is the extracted heat from the hot heat bath. In the case that the heat baths' particle are uncorrelated each others, we can construct a specific work extraction whose efficiency coincides with the upper bound up to the term of the first order q_n in general cases, and up to the term of the second order q_n^2 in the case that $Q_{H,n}$ is non-decreasing of n,; namely, thermodynamics gives an approximation to the optimal efficiency which is accurate up to the the order of q_n in general, and up to the order of q_n^2 in the case that $Q_{H,n}$ is non-decreasing of n, respectively.

The present thesis is organized as follows. In Chapter 2, we review the previous results which are closely related to our results. In Chapter 2 particulary in Subsection 2.3, we also review three of the author's results, which give the entanglement description of the information thermodynamics. They correspond to Refs. [28–30]. In Chapter 3, we reconsider the formulation of heat engines, and give the work extraction as a measurement process. The results in Chapter 3 is based on Ref. [39] under collaboration with Prof. M. Hayashi. In Chapter 4, we give a theory of the efficiency of heat engines in mesoscopic scale. The results in Chapter 4 are based on Ref. [40] under collaboration with Prof. M. Hayashi. In Chapter 5, we summarize the present thesis, and discuss future works. In Appendix A, we give the detail of a lemma in Subsection 2.3. In Appdendix B, we give one of the author's results, which corresponds to Ref. [62]. It gives a necessary and sufficient condition for the possibility of deterministic LOCC transformation and is used in Appendix A.

Chapter 2

Review of Thermodynamics in Quantum systems

Various approaches have been devised for statistic analyses of the quantum heat engines.

These studies model the heat engines and the heat baths as a mass of quantum particles, and analyze their thermodynamic features. In the present chapter, we review the studies focusing on the work extraction from quantum heat engines.

2.1 Statistic derivation of principle of maximum work

In Sections 2.1, 2.2 and 2.3, we review the semi-classical work extraction scenario [8–10, 25–30]. In this scenario, we consider the work extraction from quantum systems by a classical external system; we assume the energy loss of the internal system under a unitary time evolution to be the extracted work. Under the assumption, Tasaki derived the principle of the maximum work in 2000 [8]. In the present section, we review the derivation.

As the set up, let us consider a thermodynamic system S that is in contact with a heat bath B at temperature T. We express the Hamiltonian of the whole system as

$$\hat{H}(\vec{\lambda}(t)) = \hat{H}^S(\vec{\lambda}^S(t)) + \hat{H}^{SB}(\vec{\lambda}^{SB}(t)) + \hat{H}^B, \tag{2.1}$$

where the first term is the Hamiltonian of the system S, the third term is that of the bath B, the second term is the interaction Hamiltonian between the system them, and where $\vec{\lambda}^S(t)$ and $\vec{\lambda}^{SB}(t)$ are the external paramters.

In the above setup, we perform a thermodynamic operation as a unitary time evolution. We control the external parameters time-dependently, and perform the unitary time evolution $U = T_{\rightarrow}\exp(-i\int H(\vec{\lambda}(t))dt)$ on the composit system SB, from $t = 0$ to $t = \tau$. We assume that the system S is detached from B initially and finally; $H_{SB}(\vec{\lambda}_{SB}(0)) = H_{SB}(\vec{\lambda}_{SB}(\tau)) = 0$. We also assume that the initial state ρ_i of SB is the Gibbs state at the inverse temperature $\beta := 1/k_BT$;

$$\hat{\rho}_\mathrm{i} = \frac{\exp(-\beta\hat{H}^S_\mathrm{i})}{Z^S(H^S_\mathrm{i},\beta)} \otimes \frac{\exp(-\beta\hat{H}^B)}{Z^B(\beta)}, \tag{2.2}$$

where $\hat{H}^S_\mathrm{i} = \hat{H}^S(\vec{\lambda}^S(0))$, $Z^S(H^S_\mathrm{i},\beta) = \mathrm{tr}[\exp(-\beta\hat{H}^S)]$ and $Z^B = \mathrm{tr}[\exp(-\beta\hat{H}^B)]$.

During the time evolution, the energy is transmitted to the external operator through the back reaction of the control parameter, and we assume the energy loss to be the extracted work:

$$W(U) := \mathrm{tr}[\hat{H}_{\mathrm{i}}\rho_{\mathrm{i}} - \hat{H}_{\mathrm{f}}\rho_{\mathrm{f}}], \tag{2.3}$$

where $\hat{H}_{\mathrm{i}} := \hat{H}_{\mathrm{i}}^S + \hat{H}^B$, $\hat{H}_{\mathrm{f}} := \hat{H}^S(\vec{\lambda}^S(\tau)) + \hat{H}^B$ and $\rho_{\mathrm{f}} := U\rho_{\mathrm{i}}U^\dagger$. We further assume that we can realize a thermodynamic equilibrium state at temperature T by connecting S and B and waiting.

Then, as we show below, the principle maximum work holds:

$$W(U) \leq -\Delta F^S(\beta), \tag{2.4}$$

where

$$\begin{aligned}
\Delta F^S(\beta) &:= F^S(H_{\mathrm{f}}^S, \beta) - F^S(H_{\mathrm{i}}^S, \beta), &(2.5)\\
F^S(H^S, \beta) &:= -\frac{1}{\beta}\log Z^S(H^S, \beta). &(2.6)
\end{aligned}$$

Note that the Helmholtz free energy $F^S(H_{\mathrm{f}}, \beta)$ does not depend on the final state ρ_{f}. Since we have assume that we can realize a thermodynamic equilibrium state at temperature T by connecting S and B and waiting, we can regard $F(H_{\mathrm{f}}, \beta)$ as the Helmholtz free energy of the final state. The equilibrium state may not be the Gibbs state, but just a macroscopic equilibrium state. In the subsections 2.2 and 2.3, we need the assumption in order to treat $F(H_{\mathrm{f}}, \beta)$ as the Helmholtz free energy of the final state. Because this assumption is not related to the proof of (2.13), the inequality (2.4) holds whether the assumption holds or not.

Proof: Note that for an arbitrary Gibbs state $\rho_{\mathrm{G},\beta}(H) := \exp(-\beta H)/Z(H,\beta)$ with an arbitrary Hamiltonian H, the following equality holds;

$$H = -\frac{1}{\beta}\log \rho_{\mathrm{G},\beta}(H) + F(H, \beta). \tag{2.7}$$

Using (2.7) and $S(\rho) := -\mathrm{tr}[\rho\log\rho]$, we convert $W(U)$ in (2.3) as follows;

$$\begin{aligned}
W(U) &:= \mathrm{tr}[\hat{H}_{\mathrm{i}}\rho_{\mathrm{i}} - \hat{H}_{\mathrm{f}}\rho_{\mathrm{f}}] &(2.8)\\
&\overset{(a)}{=} \mathrm{tr}\left[\left(-\frac{1}{\beta}\log\rho_{\mathrm{i}} + F(H_{\mathrm{i}},\beta)\right)\rho_{\mathrm{i}} - \left(-\frac{1}{\beta}\log\rho_{\mathrm{G},\beta}(H_{\mathrm{f}}) + F(H_{\mathrm{f}},\beta)\right)\rho_{\mathrm{f}}\right] &(2.9)\\
&= \frac{1}{\beta}S(\rho_{\mathrm{i}}) + F(H_{\mathrm{i}},\beta) - F(H_{\mathrm{f}},\beta) + \frac{1}{\beta}\mathrm{tr}[\rho_{\mathrm{f}}\log\rho_{\mathrm{G},\beta}(H_{\mathrm{f}})] &(2.10)\\
&\overset{(b)}{=} \frac{1}{\beta}S(\rho_{\mathrm{i}}) + F(H_{\mathrm{i}},\beta) - F(H_{\mathrm{f}},\beta) - \frac{1}{\beta}S(\rho_{\mathrm{f}}) - \frac{1}{\beta}D(\rho_{\mathrm{f}}\|\rho_{\mathrm{G},\beta}(H_{\mathrm{f}})) &(2.11)\\
&= \frac{1}{\beta}S(\rho_{\mathrm{i}}) + F^S(H_{\mathrm{i}}^S,\beta) + F^B(H^B,\beta) - F^S(H_{\mathrm{f}}^S,\beta) - F^B(H^B,\beta) - \frac{1}{\beta}S(\rho_{\mathrm{f}}) - \frac{1}{\beta}D(\rho_{\mathrm{f}}\|\rho_{\mathrm{G},\beta}(H_{\mathrm{f}}))\\
&= \frac{1}{\beta}(S(\rho_{\mathrm{i}}) - S(\rho_{\mathrm{f}})) - \Delta F^S(\beta) - \frac{1}{\beta}D(\rho_{\mathrm{f}}\|\rho_{\mathrm{G},\beta}(H_{\mathrm{f}})) &(2.12)\\
&\overset{(c)}{\leq} \frac{1}{\beta}(S(\rho_{\mathrm{i}}) - S(\rho_{\mathrm{f}})) - \Delta F^S(\beta), &(2.13)
\end{aligned}$$

where $D(\rho\|\sigma) := \mathrm{Tr}[\rho(\log\rho - \log\sigma)]$, and where the equality (a) follows from (2.7), the equality (b) follows from $\mathrm{tr}[\rho\log\sigma] = -S(\rho) - D(\rho\|\sigma)$, and the inequality (c) follows from $D(\rho\|\sigma) \geq 0$. Because of $S(\rho_{\mathrm{i}}) = S(\rho_{\mathrm{f}})$, the inequality (2.13) yields (2.4). $\square$

2.2 Information Thermodynamics

2.2.1 Second law with feedback control

In 2008, Sagawa and Ueda extended the above derivation of the principle of maximum work and derived an extended second law for the thermodynamic operation with feedback control [25]. In the present subsection, we review the result in Ref. [25].

We use the same setup as in the section 2.1[1] and perform the isothermal operation with feedback control as follows.

Isothermal operation with feedback control

Step 1: We control the external parameter $\vec{\lambda}(t)$ of the Hamiltonian (2.1) and perform the thermodynamic operation $U := T_{\rightarrow}\exp(-i\int H(\vec{\lambda}(t))dt)$ on the initial state (2.2) of the composit system SB. When Step 1 finishes, the state of SB becomes $\rho_1 := U\rho_{\mathrm{i}}U^{\dagger}$.

Step 2: We perform a CP-instrument $\{\mathcal{E}_j\}$ on S, where each $\mathcal{E}_j$ is a complete positive map, and $\sum_j \mathcal{E}_j$ is a completely positive and trace preserving(CPTP) map. When Step 2 finishes, the state of SB becomes $\rho_2^j := \mathcal{E}_j(\rho_1)/p_j$ with probability $p_j := \mathrm{tr}[\mathcal{E}_j(\rho_1)]$.

Step 3: We perform the feedback control $U_{(j)} := T_{\rightarrow}\exp(-i\int H(\vec{\lambda}_j(t))dt)$ depending on the outcome j of $\{\mathcal{E}_j\}$. When Step 3 finishes, the state of SB becomes $\rho_{\mathrm{f}}^j := U_{(j)}\mathcal{E}_j(\rho_1)U_{(j)}^{\dagger}/p_j$. We assume that the Hamiltonian of SB is the same for every j at the end of Step 3;

$$H_{\mathrm{f}} := H_{\mathrm{f}}^S + H^B. \tag{2.14}$$

For the above thermodynamic operation with feedback control, we define the extracted work as

$$W_{\mathrm{fb}} := \mathrm{tr}[\hat{H}_{\mathrm{i}}\rho_{\mathrm{i}} - \sum_j p_j \hat{H}_{\mathrm{f}}\rho_{\mathrm{f}}^j]. \tag{2.15}$$

Then, as we show below, the extended principle maximum work holds:

$$W_{\mathrm{fb}} \leq -\Delta F^S(\beta) + \frac{1}{\beta}I_{\mathrm{QC}}, \tag{2.16}$$

where

$$I_{\mathrm{QC}} := S(\rho_1) - \sum_j p_j S(\rho_2^j). \tag{2.17}$$

The quantity I_{QC} was introduced by Sagawa and Ueda, and called the QC-mutual information content. Sagawa and Ueda pointed out that the QC-mutual information content I_{QC} satisfies the following features and defined I_{QC} as the information content obtained by the measurement $\{\mathcal{E}_j\}$;

- When the measurement $\{\mathcal{E}_j\}$ is classical, i.e., for the spectral decomposition $\rho_1 = \sum_i q_i|\psi_i\rangle\langle\psi_i|$ with or-

[1] In Ref. [25], Sagawa and Ueda treat not only one heat bath B, but also many heat baths $\{B_m\}_{m=1}^n$. However, the essence can be seen in the case of $n=1$, and thus we treat only the case of $n=1$ for simplicity.

thonormal basis $\{|\psi_i\rangle\}_i$, each CP-map $\mathcal{E}_j$ satisfies

$$\mathcal{E}_j(\rho_1) = \sum_j \frac{q_{i,j}}{p_j}|\psi_{i|j}\rangle\langle\psi_{i|j}|, \text{ where } q_{i,j} := \mathrm{tr}[\mathcal{E}_j(|\psi_i\rangle\langle\psi_i|)] \tag{2.18}$$

with proper orthonomal basis $\{|\psi_{i|j}\rangle\}_i$, I_{QC} reduces to the classical mutual information;

$$I_{\mathrm{QC}} = \sum_{i,j} q_{i,j} \log \frac{q_{i,j}}{q_i p_j}. \tag{2.19}$$

- The QC-mutual information content I_{QC} depends only on the premeasurement state ρ_1 and the CP-instrument $\{\mathcal{E}_j\}$.

From the above point of view, the inequality (2.16) means that in the thermodynamic processes with feedback control, the extracted work can exceed the conventional second law by the amount of the information extracted by the measurement. Note that the quantity I_{QC} is determined when the measurement is finished. Regardless of the feedback control $\{U_j\}$, the surplus $W_{\mathrm{fb}} - (-\Delta F)$ is bounded by the QC-mutual information I_{QC}.

Proof of (2.16)**:** In the same way as the derivation of (2.13), we can convert W_{fb} as follows;

$$\begin{aligned}
W_{\mathrm{fb}} &:= \mathrm{tr}[\hat{H}_{\mathrm{i}}\rho_{\mathrm{i}} - \sum_j p_j \hat{H}_{\mathrm{f}}\rho_{\mathrm{f}}^j] && (2.20)\\
&= \mathrm{tr}\left[\left(-\frac{1}{\beta}\log\rho_{\mathrm{i}} + F(H_{\mathrm{i}},\beta)\right)\rho_{\mathrm{i}} - \sum_j p_j \left(-\frac{1}{\beta}\log\rho_{\mathrm{G},\beta}(H_{\mathrm{f}}) + F(H_{\mathrm{f}},\beta)\right)\rho_{\mathrm{f}}^j\right] && (2.21)\\
&= \frac{1}{\beta}S(\rho_{\mathrm{i}}) + F(H_{\mathrm{i}},\beta) - \sum_j p_j \left(F(H_{\mathrm{f}},\beta) - \frac{1}{\beta}\mathrm{tr}[\rho_{\mathrm{f}}^j \log\rho_{\mathrm{G},\beta}(H_{\mathrm{f}})]\right) && (2.22)\\
&= \frac{1}{\beta}S(\rho_{\mathrm{i}}) + F(H_{\mathrm{i}},\beta) - \sum_j p_j \left(F(H_{\mathrm{f}},\beta) + \frac{1}{\beta}S(\rho_{\mathrm{f}}^j) + \frac{1}{\beta}D(\rho_{\mathrm{f}}^j\|\rho_{\mathrm{G},\beta}(H_{\mathrm{f}}))\right) && (2.23)\\
&= \frac{1}{\beta}S(\rho_{\mathrm{i}}) + F^S(H_{\mathrm{i}}^S,\beta) + F^B(H^B,\beta)\\
&\quad \sum_j p_j \left(F^S(H_{\mathrm{f}}^S,\beta) + F^B(H^B,\beta) + \frac{1}{\beta}S(\rho_{\mathrm{f}}^j) + \frac{1}{\beta}D(\rho_{\mathrm{f}}^j\|\rho_{\mathrm{G},\beta}(H_{\mathrm{f}}))\right)\\
&= \frac{1}{\beta}I_{\mathrm{QC}} - \Delta F^S(\beta) - \frac{1}{\beta}\sum_j p_j D(\rho_{\mathrm{f}}^j\|\rho_{\mathrm{G},\beta}(H_{\mathrm{f}})) && (2.24)\\
&\leq -\Delta F^S(\beta) + \frac{1}{\beta}I_{\mathrm{QC}}. && (2.25)
\end{aligned}$$

□

2.2.2 Lower bounds of energy costs for information processes

In the subsection 2.2.1, we derived an upper bound of the extracted work of a thermodynamic operation with feedback control. The essence of the derivation was the relations (2.7) and $\mathrm{tr}[\rho\log\sigma] = -S(\rho) - D(\rho\|\sigma)$. By using these two relations, Sagawa and Ueda also derived a lower bound of energy costs for a measurement and an information erase [27]. In the present subsection, we review the result in Ref. [27].

As the setup, let us consider a thermodynamic system S and a memory M which is connected to a heat bath B_M. The thermodynamic system S is the target of the measurement. The memory M stores the information on the outcomes of the measurement. The heat bath B_M is at a temperature T and is in contact with M.

In order to use M as the memory, we divide $\mathbf{H}^M$, which is the Hilbert space of M, into mutually orthogonal subspaces $\mathbf{H}^M_{(k)}$ $(k = 0, ..., N)$, where the subscripts k specify the measurement outcomes; $\mathbf{H}^M = \oplus_{k=0}^N \mathbf{H}^M_{(k)}$. We consider the outcome k to be stored in M when the support of the density operator of M is in $\mathbf{H}^M_{(k)}$. Without losing generality, we can assume that $k = 0$ corresponds to the standard state of M.

In order to consider a measurement process and an information erase process as isothermal processes, we assume that the memory M and the heat bath B_M keep interacting with each other during these processes. In each process, the Hamiltonian of the composit system MB_M is written as follows;

$$\hat{H}^{MB}_{\mathrm{meas}}(t) = \hat{H}^M_{\mathrm{meas}}(t) + \hat{H}^{\mathrm{int}}_{\mathrm{meas}}(t) + \hat{H}^{B_M}, \tag{2.26}$$

$$\hat{H}^{MB}_{\mathrm{eras}}(t) = \hat{H}^M_{\mathrm{eras}}(t) + \hat{H}^{\mathrm{int}}_{\mathrm{eras}}(t) + \hat{H}^{B_M}, \tag{2.27}$$

where $\hat{H}^{\mathrm{int}}_{\mathrm{meas}}(t)$ and $\hat{H}^{\mathrm{int}}_{\mathrm{eras}}(t)$ are the interaction Hamiltonians between M and B. We consider the measurement process from $t = t^{\mathrm{meas}}_{\mathrm{ini}}$ to $t = t^{\mathrm{meas}}_{\mathrm{fin}}$ and the erase process from $t = t^{\mathrm{eras}}_{\mathrm{ini}}$ to $t = t^{\mathrm{eras}}_{\mathrm{fin}}$. At the initial and final times of the processes, the Hamiltonians $\hat{H}^{\mathrm{int}}_{\mathrm{meas}}(t)$ and $\hat{H}^{\mathrm{int}}_{\mathrm{eras}}(t)$ become $\hat{0}$, and the the Hamiltonians $\hat{H}^M_{\mathrm{meas}}(t)$ and $\hat{H}^M_{\mathrm{eras}}(t)$ become $\oplus_k \hat{H}^M_{(k)} := \oplus_k \sum_i \epsilon_{ki} |\epsilon_{ki}\rangle\langle\epsilon_{ki}|$, where $\{|\epsilon_{ki}\rangle\}_i$ is an orthonormal basis of $\mathbf{H}^M_{(k)}$.

Under the above setup, we consider the measurement process and the information erase process as follows:

Measurement Process

Initial state At $t = t^{\mathrm{meas}}_{\mathrm{ini}}$, the composit system SMB_M is in the following initial state:

$$\rho^{\mathrm{m}}_{\mathrm{i}} \equiv \rho^S_{\mathrm{ini}} \otimes \rho_{\mathrm{G},\beta}(H^M_0) \otimes \rho_{\mathrm{G},\beta}(H^{B_M}). \tag{2.28}$$

Note that ρ^S_{ini} is an arbitrary state of S.

Step M1 As the former part of the measurement on S, we perform a unitary transformation $\hat{U}_{SMB_M}$ on SMB_M from $t = t^{\mathrm{meas}}_{\mathrm{ini}}$ to $t = t^{\mathrm{meas}}_1$. When Step M1 is completed, the state of SMB_M becomes $\rho^{\mathrm{m}}_1 := U_{SMB_M} \rho^{\mathrm{m}}_{\mathrm{i}} U^\dagger_{SMB_M}$.

Step M2 As the latter part of the measurement on S, we perform a projective measurement $\hat{P}_{(k)} \equiv \sum_i |\epsilon_{ki}\rangle\langle\epsilon_{ki}|$ on M from $t = t^{\mathrm{meas}}_1$ to $t = t^{\mathrm{meas}}_2$. When Step M2 is completed, the state of SMB_M becomes $\rho^{\mathrm{m}}_{(k),2} := P_{(k)} \rho^{\mathrm{m}}_1 P_{(k)} / p_{(k)}$ with the probability $p_{(k)} := \mathrm{tr}[P_{(k)} \rho^{\mathrm{m}}_1 P_{(k)}]$. We also assume that each $\rho^{\mathrm{m}}_{(k),2}$ does not have the correlation between S and MB; namely, $\rho^{\mathrm{m}}_{(k),2} = \rho^S_{(k)} \otimes \rho^{MB_M}_{(k)}$ holds, where $\rho^S_{(k)} := \mathrm{tr}_{MB_M}[\rho^{\mathrm{m}}_{(k),2}]$ and $\rho^{MB_M}_{(k)} := \mathrm{tr}_S[\rho^{\mathrm{m}}_{(k),2}]$.

Energy cost We introduce the average energy cost W^M_{meas} which is necessary for the measurement process as

$$W^M_{\mathrm{meas}} \equiv \sum_k p_k \mathrm{tr}[\rho^{MB}_{(k)} (\hat{H}^M_k + \hat{H}^{B_M})] - \mathrm{tr}[\rho_{\mathrm{G},\beta}(H^M_0) \otimes \rho_{\mathrm{G},\beta}(H^{B_M})(\hat{H}^M_0 + \hat{H}^{B_M})]. \tag{2.29}$$

We also define the average difference of the Helmholtz free energy:

$$\Delta F^M_{\mathrm{meas}} \equiv \sum_k p_{(k)} F(H^M_k, \beta) - F(H^M_0, \beta). \tag{2.30}$$

Information Erase Process

Initial state At $t = t^{\rm eras}_{\rm ini}$, the composit system MB_M is in $\rho^{\rm e}_{\rm i} := \sum_k p_{(k)}\rho^{\rm e}_{(k)}$, where $\rho^{{\rm e}M}_{(k)} = {\rm tr}_{B_M}[\rho^{\rm e}_{(k)}]$ belongs to $\mathbf{H}^M_k$ for each k.

Step E1 From $t = t^{\rm eras}_{\rm ini}$ to $t = t^{\rm eras}_{\rm fin}$, we perform the unitary transformation U_{MB_M} such that ${\rm tr}[P_{(k)}\rho^{\rm e}_{\rm f}] = 0$ for any $k \neq 0$, where $\rho^{\rm e}_{\rm f} := U_{MB_M}\rho^{\rm e}_{\rm i}U^\dagger_{MB_M}$.

Energy cost We define the energy cost which is necessary for the above process as

$$W^M_{\rm eras} \equiv {\rm tr}[\rho^{\rm e}_{\rm f}(\hat{H}^M + \hat{H}^{B_M})] - {\rm tr}[\rho^{\rm e}_{\rm i}(\hat{H}^M + \hat{H}^{B_M})]. \tag{2.31}$$

We also define the average change of the Helmholtz free energy as

$$\Delta F^M_{\rm eras} \equiv F(H^M_0, \beta) - \sum_k p_k F(H^M_k, \beta). \tag{2.32}$$

For the above two information processes, the following three inequalities hold;

$$W^M_{\rm meas} \geq \Delta F^M_{\rm meas} + \frac{1}{\beta}(I_{\rm QC} - H\{p_{(k)}\}), \tag{2.33}$$

$$W^M_{\rm eras} \geq -\Delta F^M_{\rm eras} + \frac{1}{\beta}H\{p_{(k)}\} \quad \text{if} \ \ \rho^{\rm e}_{(k)} = \rho_{{\rm G},\beta}(H^M_k + H^{B_M}), \tag{2.34}$$

$$W^M_{\rm meas} + W^M_{\rm eras} \geq \frac{1}{\beta}I_{\rm QC} \qquad \text{if} \ \ \rho^{\rm e}_{(k)} = \rho^{\rm m}_{(k),2}. \tag{2.35}$$

where

$$I_{\rm QC} := S(\rho^S_{\rm ini}) - \sum_k p_k S(\rho^S_{(k)}), \tag{2.36}$$

$$H\{p_{(k)}\} := -\sum_k p_{(k)} \log p_{(k)}. \tag{2.37}$$

By combining (2.16) and (2.35), we recover the second law of the total system is recovered;

$$W_{\rm tot} := W(U, \{\mathcal{E}_j, U_j\}) - W^M_{\rm meas} - W^M_{\rm eras} \leq -\Delta F^S(\beta) = -\Delta F^{SM}(\beta). \tag{2.38}$$

Proof: We first prove (2.33). In the same way as the derivations of (2.13) and (2.25), we can convert $W^M_{\rm meas}$ as follows;

$$\begin{aligned}
W^M_{\rm meas} &\equiv \sum_k p_k {\rm tr}[\rho^{MB}_{(k)}(\hat{H}^M_k + \hat{H}^B)] - {\rm tr}[\rho_{{\rm G},\beta}(H^M_0) \otimes \rho_{{\rm G},\beta}(H^{B_M})(\hat{H}^M_0 + \hat{H}^B)] && (2.39)\\
&= \sum_k p_k {\rm tr}[\rho^{MB}_{(k)}(-\frac{1}{\beta}\log \rho_{{\rm G},\beta}(\hat{H}^M_k + \hat{H}^B) + F(H^M_k, \beta) + F(H^B, \beta))] \\
&\quad -{\rm tr}[\rho_{{\rm G},\beta}(H^M_0 + H^{B_M})(-\frac{1}{\beta}\log \rho_{{\rm G},\beta}(\hat{H}^M_0 + \hat{H}^B) + F(H^M_0, \beta) + F(H^M, \beta)] && (2.40)\\
&= \Delta F^M_{\rm meas} + \frac{1}{\beta}\left(\sum_k p_k S(\rho^{MB_M}_k) - S(\rho_{{\rm G},\beta}(H^M_0 + H^{B_M}))\right) \\
&\quad +\frac{1}{\beta}\sum_k p_k D(\rho^{MB}_{(k)} \| \rho_{{\rm G},\beta}(\hat{H}^M_k + \hat{H}^B)) && (2.41)\\
&\geq \Delta F^M_{\rm meas} + \frac{1}{\beta}\left(\sum_k p_k S(\rho^{MB_M}_k) - S(\rho_{{\rm G},\beta}(H^M_0 + H^{B_M}))\right). && (2.42)
\end{aligned}$$

Thus, in order to prove (2.33), we only have to prove the following inequality;

$$\sum_k p_k S(\rho_k^{MB_M}) - S(\rho_{\mathrm{G},\beta}(H_0^M + H^{B_M})) \geq I_{\mathrm{QC}} - H\{p_{(k)}\}. \tag{2.43}$$

We obtain (2.43) as follows;

$$\begin{aligned}
& \sum_k p_k S(\rho_k^{MB_M}) - S(\rho_{\mathrm{G},\beta}(H_0^M + H^{B_M})) - I_{\mathrm{QC}} + H\{p_{(k)}\} && (2.44)\\
\overset{(a)}{=} & \sum_k p_k S(\rho_k^{MB_M}) - S(\rho_{\mathrm{G},\beta}(H_0^M + H^{B_M})) + \sum_k p_k S(\rho_{(k)}^S) - S(\rho_{\mathrm{ini}}^S) + H\{p_{(k)}\} && (2.45)\\
\overset{(b)}{=} & \sum_k p_k S(\rho_k^{MB_M} \otimes \rho_{(k)}^S) - S(\rho_{\mathrm{G},\beta}(H_0^M + H^{B_M}) \otimes \rho_{\mathrm{ini}}^S) + H\{p_{(k)}\} && (2.46)\\
\overset{(c)}{=} & \sum_k p_k S(\rho_{(k),2}^{\mathrm{m}}) - S(\rho_{\mathrm{i}}^{\mathrm{m}}) + H\{p_{(k)}\} && (2.47)\\
\overset{(d)}{=} & S(\sum_k p_k \rho_{(k),2}^{\mathrm{m}}) - S(\rho_{\mathrm{i}}^{\mathrm{m}}) = S(\sum_k P_k \rho_1^{\mathrm{m}} P_k) - S(\rho_1^{\mathrm{m}}) \geq 0, && (2.48)
\end{aligned}$$

where the equality (a) follows from the definition of I_{QC}, the equality (b) follows from $S(\rho\otimes\sigma) = S(\rho) + S(\sigma)$, the equality (c) follows from the assumption $\rho_{(k),2}^{\mathrm{m}} = \rho_{(k)}^{MB_M} \otimes \rho_{(k)}^S$, and the equality (d) follows from the fact that $S(\sum_k p_k \rho_k) = H\{p_k\} + \sum_k p_k S(\rho_k)$ holds when the supports of ρ_k are orthogonal to each other.

Next, we prove (2.34) and (2.35). In the same way as the derivation of (2.42), we can convert W_{eras}^M as follows;

$$\begin{aligned}
W_{\mathrm{eras}}^M &= \Delta F_{\mathrm{eras}}^M + \frac{1}{\beta}\left(S(\rho_{\mathrm{f}}^{\mathrm{e}}) - \sum_k p_k S(\rho_{(k)}^{\mathrm{e}})\right)\\
&\quad + \frac{1}{\beta} D(\rho_{\mathrm{f}}^{\mathrm{e}} \| \rho_{\mathrm{G},\beta}(H_0^M + H^{B_M})) - \frac{1}{\beta}\sum_k p_k D(\rho_{(k)}^{\mathrm{e}} \| \rho_{\mathrm{G},\beta}(H_k^M + H^{B_M})). && (2.49)
\end{aligned}$$

Because the supports of $\rho_{(k)}^{\mathrm{e}}$ are orthogonal to each other, the following equation holds;

$$\begin{aligned}
S(\rho_{\mathrm{f}}^{\mathrm{e}}) - \sum_k p_k S(\rho_{(k)}^{\mathrm{e}}) &= S(\sum_k p_k U_{MB} \rho_{(k)}^{\mathrm{e}} U_{MB}^\dagger) - \sum_k p_k S(\rho_{(k)}^{\mathrm{e}}) && (2.50)\\
&= H\{p_k\} + \sum_k p_k S(U_{MB} \rho_{(k)}^{\mathrm{e}} U_{MB}^\dagger) - \sum_k p_k S(\rho_{(k)}^{\mathrm{e}}) = H\{p_k\}. && (2.51)
\end{aligned}$$

Thus,

$$W_{\mathrm{eras}}^M \geq \Delta F_{\mathrm{eras}}^M + \frac{1}{\beta} H\{p_k\} - \frac{1}{\beta}\sum_k p_k D(\rho_{(k)}^{\mathrm{e}} \| \rho_{\mathrm{G},\beta}(H_k^M + H^{B_M})) \tag{2.52}$$

holds. When $\rho_{(k)}^{\mathrm{e}} = \rho_{\mathrm{G},\beta}(H_k^M + H^{B_M})$ holds, (2.52) clearly yields (2.34), because of $D(\rho_{(k)}^{\mathrm{e}} \| \rho_{\mathrm{G},\beta}(H_k^M + H^{B_M})) = 0$. When $\rho_{(k)}^{\mathrm{e}} = \rho_{(k),2}^{\mathrm{m}}$ holds, then (2.35) follows from (2.41), (2.43) and (2.52). □

2.3 Entanglement Description of Information Thermodynamics

In the previous section 2.2, we have reviewed the information thermodynamics which was given by Sagawa and Ueda [25,27]. The point is the following two statements. In the thermodynamic processes with feedback control, the extracted work can exceed the conventional second law by the product of the temperature and the amount of the information extracted by the measurement, which is measured by the QC-mutual information $I_{\rm QC}$. On the other hand, the sum of the energy costs for the measurement and the information erase is larger than or equal to the product.

The QC-mutual information content $I_{\rm QC}$ is determined when the measurement process is completed. However, the measurement process consists of the two steps: the first step is the unitary interaction U between the system S and the memory M; the second step is the projective measurement on the memory M. Because the second step is independent of the time evolution of S, the information extraction in the measurement process must be finished at the end of the first step. Based on the above consideration, the author has defined the amount of the entanglement gain which is caused by the unitary interaction U between the system S and the memory M, in 2013 [28]. We can understand the amount of the entanglement gain as the "fresh" information and also understand the projective measurement on the memory as an interpretation process of the fresh information.

In the present section, we review the author's results in Refs. [28–30]: we define the amount of the entanglement gain [28, 30] in Subsection 2.3.1; we give an upper bound of the extracted work of the information thermodynamic process with the entanglement gain [28] in Subsection 2.3.2; we give an lower bound for the energy cost of the information processes [29] in Subsection 2.3.3. The difference between the entanglement gain and $I_{\rm QC}$ is clear especially in the bounds for the energy cost of information processes; the bounds with the entanglement gain are strictly tighter than (2.33), (2.34) and (2.35). This fact stands for the essential irreversibility of the information thermodynamics. In particular, when the measurement is not classical, the sum of the energy costs for the measurement and the information erase is strictly larger than the energy profit by the feedback control.

2.3.1 Entanglement transfer during the measurement

When we perform the CP-instrument $\{\mathcal{E}_j\}$ on the system A, the premeasurement state ρ^A changes to the state $\mathcal{E}_j(\rho^A)/p_j$ with the probability $p_j := \mathrm{tr}[\mathcal{E}_j(\rho^A)]$. We also take a proper reference system R to have a proper pure state $|\psi_{AR}\rangle$ such that $\mathrm{tr}_R[|\psi_{AR}\rangle\langle\psi_{AR}|] = \rho_A$. Then, we define the entanglement gain $-\Delta E_F^{A-R}$ as follows;

$$-\Delta E_F^{A-R} := E_F^{A-R}(|\psi_{AR}\rangle\langle\psi_{AR}|) - E_F^{A-R}(\sum_j \mathcal{E}_j \otimes \hat{1}_R(|\psi_{AR}\rangle\langle\psi_{AR}|)), \tag{2.53}$$

where $E_F^{A\text{-}R}(\hat{\rho})$ is the entanglement of formation [54] between A and R;

$$E_F^{A\text{-}R}(\hat{\rho}) \equiv \min_{\hat{\rho}=\sum q_l|\phi^l\rangle\langle\phi^l|} \sum_l q_l E^{A\text{-}R}(|\phi^l\rangle) \tag{2.54}$$

with $E^{A\text{-}R}(|\phi^l\rangle)$ being the entanglement entropy [53] between A and R for a pure state $|\phi^l\rangle$.

Let us see that the quantity $-\Delta E_F^{A-R}$ means the amount of the entanglement gain. Let the set $(\mathcal{H}_\mathcal{M}, \rho_M, U, \{P_j\})$ be the indirect measurement model which yields the CP-instrument $\{\mathcal{E}_j\}$. We also take another reference system R_M to obtain a proper pure state $|\phi_{MR_M}\rangle$ such that $\mathrm{tr}_{R_M}[|\phi_{MR_M}\rangle\langle\phi_{MR_M}|] = \rho_M$. Then, the premeasurement state of the total system is given by

$$|\psi_{AR}\rangle \otimes |\phi_{MR_M}\rangle. \tag{2.55}$$

Because of

$$\sum_j \mathcal{E}_j \otimes \hat{1}_R(|\psi_{AR}\rangle\langle\psi_{AR}|) = \mathrm{tr}_{MR_M}[U(|\psi_{AR}\rangle \otimes |\phi_{MR_M}\rangle\langle\psi_{AR}| \otimes \langle\phi_{MR_M}|)U^\dagger], \tag{2.56}$$

we can express (2.53) as follows:

$$-\Delta E_F^{A\text{-}R} = E_F^{A\text{-}R}|_{\text{before } U} - E_F^{A\text{-}R}|_{\text{after } U}. \tag{2.57}$$

During the unitary interaction U between A and M which is the first half step of the measurement $\mathcal{E}_j$, the amount of the entanglement between AM and MR_M does not change, because the entanglement does not change by the local unitary transformation. On the other hand, the quantity $-\Delta E_F^{A-R}$ is the loss of entanglement between A and R, which is caused by U. Thus, we can interpret $-\Delta E_F^{A-R}$ as the amount of the entanglement gain which is taken from the system A by the memory M during the interaction U.

Because $-\Delta E_F^{A-R}$ is defined by $\{\mathcal{E}_j\}$, the indirect measurement models which yield the same CP-instrument all produce the same value of $-\Delta E_F^{A-R}$. Namely, the measurements whose QC-mutual informations are the same have the same value of $-\Delta E_F^{A-R}$. However, the converse does not hold. Because $-\Delta E_F^{A-R}$ does not depend on the projective measurement $\{P_j\}$ of the indirect measurement model $(\mathcal{H}_\mathcal{M}, \rho_M, U, \{P_j\})$, there exist many measurements whose entanglement gains are the same, but whose QC-mutual informations are different. In fact, the following lemma shows that the entanglement gain is the upper limit of the QC-mutual information.

Lemma 1. *For an arbitrary measurement $\{\mathcal{E}_j\}$, the following inequality holds:*

$$I_{\mathrm{QC}} \leq -\Delta E_F^{SB-R}. \tag{2.58}$$

The equality of the inequality (2.58) *is achieved when we perform the "best" measurement on the memory. Namely, there exists an indirect measurement model $(\mathcal{H}_\mathcal{M}, \rho_M, U, \{P_j\})$ and a proper projective measurement $\{P'_j\}$ such that $(\mathcal{H}_\mathcal{M}, \rho_M, U, \{P_j\})$ yields $\{\mathcal{E}_j\}$ and $(\mathcal{H}_\mathcal{M}, \rho_M, U, \{P'_j\})$ satisfies the equality of the inequality* (2.58)*.*

The above lemma brings a very reasonable understanding of the information gain during the measurement process. The information gain in the measurement process is finished before the end of the interaction between the system and the memory. (Note that the entanglement gains of $(\mathcal{H}_\mathcal{M}, \rho_M, U, \{P_j\})$ and $(\mathcal{H}_\mathcal{M}, \rho_M, U, \{P'_j\})$ are the same.) However, in order to make the "fresh" information comprehensible to the classical observer, we have to perform the projective measurement on the memory and obtain the classical outcome with the probabilistic distribution. The entanglement gain expresses the amount of the fresh information, whereas the QC-mutual information expresses the amount of the comprehended information.

Proof of Lemma 1: Let us take an arbitrary CP-instrument $\{\mathcal{E}_j\}$ and the indirect measurement model $(\mathcal{H}_\mathcal{M}, |0_M\rangle\langle 0_M|, U, \{P_j\})$ which yields $\{\mathcal{E}_j\}$. When we perform the CP-instrument $\{\mathcal{E}_j\}$ on S, the premeasurement state ρ_1 of SB becomes $\rho_2^j := \mathcal{E}_j(\rho_1)/p_j$ with the probability $p_j := \mathrm{tr}[\mathcal{E}_j(\rho)]$. We take the reference system R and the pure state $|\psi_{SBR}\rangle$ of SBR such that $\mathrm{tr}_R[|\psi_{SBR}\rangle\langle\psi_{SBR}|] = \rho_1$ We also define

$$\rho_2^{SBR} := \sum_j \mathcal{E}_j \otimes \hat{1}_R(|\psi_{SBR}\rangle\langle\psi_{SBR}|) = \mathrm{tr}_M[U(|\psi_{SBR}\rangle \otimes |0_M\rangle\langle\psi_{SBR}| \otimes \langle 0_M|)U^\dagger]. \tag{2.59}$$

We first prove the inequality (2.58). Because of $S(\rho_1) = E_F^{SB-R}(|\psi_{SBR}\rangle\langle\psi_{SBR}|)$ (2.17) and (2.53), the inequality (2.58) is equivalent to

$$E_F^{SB\text{-}R}(\rho_2^{SBR}) \leq \sum_j p_j S(\rho_2^j), \tag{2.60}$$

Let prove (2.60). Let us define ρ_2^{SBRj} as follows;

$$\rho_2^{SBRj} := \frac{\mathrm{tr}_M[P_j U(|\psi_{SBR}\rangle \otimes |0_M\rangle\langle\psi_{SBR}| \otimes \langle 0_M|)U^\dagger P_j]}{p_j}. \tag{2.61}$$

We also take the decomposition $\rho_2^{SBRj} = \sum_l q_l^j |\phi_l^j\rangle\langle\phi_l^j|$ such that $E_F^{SB-R}(\rho_2^{SBRj}) = \sum_l q_l^j E^{SB-R}(|\phi_l^j\rangle\langle\phi_l^j|)$. Then, $\rho_2^{SBR} = \sum_j p_j \rho_2^{SBRj} = \sum_j p_j \sum_l q_l^j |\phi_l^j\rangle\langle\phi_l^j|$ holds, and thus

$$E_F^{SB-R}(\rho_2^{SBR}) \leq \sum_j p_j E_F(\rho_2^{SBRj}) \tag{2.62}$$

holds. Note that $\rho_2^j = \sum_l q_l^j \mathrm{tr}_R[|\phi_l^j\rangle\langle\phi_l^j|]$ and that $E^{SB-R}(|\phi_l^j\rangle\langle\phi_l^j|) = S(\mathrm{tr}_R[|\phi_l^j\rangle\langle\phi_l^j|])$. Thus,

$$E_F(\rho_2^{SBRj}) = \sum_l q_l^j E^{SB-R}(|\phi_l^j\rangle\langle\phi_l^j|) = \sum_l q_l^j S(\mathrm{tr}_R[|\phi_l^j\rangle\langle\phi_l^j|]) \leq S(\sum_l q_l^j \mathrm{tr}_R[|\phi_l^j\rangle\langle\phi_l^j|]) = S(\rho_2^j). \tag{2.63}$$

holds. The inequalities (2.62) and (2.63) clearly yield (2.60).

Finally, we prove the achievability of the equality of (2.58). It is equivalent to that of (2.60). Let us take the decomposition $\rho_2^{SBR} = \sum_m r_m |\Phi_m\rangle\langle\Phi_m|$ such that $E_F^{SB-R}(\rho_2^{SBR}) = \sum_m r_m E^{SB-R}(|\Phi_m\rangle\langle\Phi_m|) = \sum_m r_m S(\rho_m)$, where $\rho_m := \mathrm{tr}_R[|\Phi_m\rangle\langle\Phi_m|]$. Because of (2.59) and because $U|\psi_{SBR}\rangle \otimes |0_M\rangle$ is pure, there exists a projective measurement $\{\tilde{P}_m\}$ such that

$$\frac{\tilde{P}_m U(|\psi_{SBR}\rangle \otimes |0_M\rangle}{|\tilde{P}_m U(|\psi_{SBR}\rangle \otimes |0_M\rangle|} = |\Phi_m\rangle. \tag{2.64}$$

Thus, $(\mathcal{H}_\mathcal{M}, |0_M\rangle\langle 0_M|, U, \{\tilde{P}_m\})$ clearly achieves the equality of (2.60). $\square$

2.3.2 Second law of information thermodynamics with entanglement gain

Because of (2.16) and Lemma 1, the following inequality[2] holds for an arbitrary thermodynamic operation with feedback control which is introduced in the subsection 2.2.1;

$$W_{\mathrm{fb}} \leq -\Delta F^S(\beta) - \frac{1}{\beta}\Delta E_F^{SB-R}. \tag{2.65}$$

The entanglement gain was given by pushing forward the idea of the QC-mutual information. The Sagawa-Ueda inequality (2.16) means that the excess $W_{\mathrm{fb}} + \Delta F$ of the extracted work over the conventional second law is bounded by the information gain I_{QC} which is obtained by the measurement. However, the excess $W_{\mathrm{fb}} + \Delta F$ can be larger when the unitary interaction between the system and the memory is finished. The inequality (2.65) expresses the bound of the excess at the end of the interaction between the system and the memory. At the time, the excess $W_{\mathrm{fb}} + \Delta F$ is bounded by the entanglement gain $-\Delta E_F^{SB-R}$ regardless of the projective measurement $\{P_j\}$ on the memory and the feedback control $\{U_j\}$. From the above point of view, the inequality

[2] In Ref. [28], the author treats not only one heat bath B, but also many heat baths $\{B_m\}_{m=1}^n$. However, the essence can be seen in the case of $n = 1$, and thus we treat only the case of $n = 1$ for simplicity.

(2.65) means that in the thermodynamic processes with feedback control, the extracted work can exceed the conventional second law by the entanglement gain of the measurement.

The condition for the achievement of the upper bound of inequality (2.65) is looser than that of the inequality (2.16). At first glance, this fact contradicts with (2.58). However, the contradiction is only spurious. Note that when the entanglement gain is determined, we can take the projective measurement $\{P_(j)\}$ on the memory freely; in other words, we can choose the "best" projective measurement. On the other hand, when the QC-mutual information is determined, $\{P_j\}$ is also determined already. Thus, the meanings of the achievability of the equalities of (2.16) and (2.65) are different. The equality of (2.16) is achievable when there exists the proper feedback $\{U_j\}$ which satisfies the equality (2.16), whereas the equality of (2.65) is achievable when there exists the proper projective measurement $\{P_j\}$ and the proper feedback $\{U_j\}$ which satisfies the equality (2.65).

Because of the achievability of the equality of (2.58), we can easily show the following corollary;

Corollary 1. *If we can always achieve the upper bound of Eq.* (2.16) *with a proper feedback* $\{\hat{U}_{(k)}\}$*, we can always achieve the upper bound of Eq.* (2.65) *with a proper set of projective measurement* $\{\hat{P}_{(k)}\}$ *and feedback* $\{\hat{U}_{(k)}\}$*.*

However, the converse of the corollary is *not* true. When we use finite systems for the heat baths, there exists the situation in which the equality of (2.65) is always achievable, but the equality of (2.16) is not achievable. We give an example of the situation in Appendix A.

2.3.3 Energy costs of the information processes

Because the excess $W_{\rm fb} + \Delta F$ of the extracted work over the conventional second law is bounded by the entanglement gain, the energy cost of the information process should be written in the entanglement gain. In fact, the lower bound of the energy cost for the measurement which are described by the entanglement gain is tighter than (2.33). To be concrete, the following inequality holds;

$$W^{M}_{\rm meas} \geq \Delta F^{M}_{\rm meas} + k_B T(-\Delta E^{S-R}_{F} - H\{p_k\}) \tag{2.66}$$

$$\geq \Delta F^{M}_{\rm meas} + k_B T(I_{\rm QC} - H\{p_k\}). \tag{2.67}$$

The equality of the inequality (2.67) is not achieved if the projective measurements on the memory are not best. This fact means that the information thermodynamics is irreversible for the most measurement $\{\mathcal{E}_k\}$; in such cases, the sum of the energy costs for the measurement and the information erase is strictly larger than the energy profit by the feedback control.

The inequality (2.66) can be shown in the same way as the proof of (2.33), by using the following lemma;

Lemma 2. *For an arbitrary density matrix* $\rho_{AA'}$ *of systems* A *and* A'*, the following inequality holds;*

$$S(\rho_A) \leq E^{A-A'}_{F}(\rho_{AA'}) + S(\rho_{AA'}), \tag{2.68}$$

where $\rho_A \equiv tr_{A'}[\rho_{AA'}]$*.*

First, we prove (2.66) by using the above Lemma.

Proof of (2.66): Because of (2.42), we only have to prove

$$\sum_k p_k S(\rho_k^{MB_M}) - S(\rho_{\mathrm{G},\beta}(H_0^M + H^{B_M})) \geq -\Delta E_F^{S-R} - H\{p_k\}. \tag{2.69}$$

In order to prove (2.69), we introduce the reference system R to have a pure state $|\psi\rangle$ of the composit system SMB_MR, which satisfies $\mathrm{tr}_R[|\psi\rangle\langle\psi|] = \rho_{\mathrm{i}}^{\mathrm{m}}$. By the unitary interaction U_{SMB_M}, the pure state $|\psi\rangle$ becomes $|\psi'\rangle := U_{SMB_M} \otimes \hat{1}_R|\psi\rangle$. By definition, $|\psi'\rangle$ satisfies $\mathrm{tr}_R[|\psi'\rangle\langle\psi'|] = \rho_1^{\mathrm{m}}$.

By applying Lemma 2 to the mixed state $\rho'_{SR} := \mathrm{tr}_{MB_M}[|\psi'\rangle\langle\psi'|]$ of SR, we obtain

$$S(\mathrm{tr}_{SMB_M}[|\psi'\rangle\langle\psi'|]) \leq E_F^{S-R}(\rho'_{SR}) + S(\rho'_{SR}). \tag{2.70}$$

Because of $\mathrm{tr}_{SMB_M}[|\psi'\rangle\langle\psi'|] = \mathrm{tr}_{SMB_M}[|\psi\rangle\langle\psi|]$, the inequality (2.70) is equivalent to

$$S(\mathrm{tr}_{SMB_M}[|\psi\rangle\langle\psi|]) \leq E_F^{S-R}(\rho'_{SR}) + S(\rho'_{SR}). \tag{2.71}$$

Because of $S(\mathrm{tr}_{SMB_M}[|\psi\rangle\langle\psi|]) = S(\mathrm{tr}_R[|\psi\rangle\langle\psi|])$, $\rho_{\mathrm{i}}^{\mathrm{m}} = \mathrm{tr}_R[|\psi\rangle\langle\psi|]$, (2.28) and (2.53), the inequality (2.71) is equivalent to

$$-\Delta E_F^{S-R} \leq S(\rho'_{SR}) - S(\rho_{\mathrm{G},\beta}(H_0^M + H^{B_M})). \tag{2.72}$$

Thus, we only have to prove

$$S(\rho'_{SR}) \leq H\{p_k\} + \sum_k p_k S(\rho_k^{MB_M}). \tag{2.73}$$

We derive (2.73) as follows

$$\begin{aligned} S(\rho'_{SR}) &\overset{(a)}{=} S(\mathrm{tr}_{SR}[|\psi'\rangle\langle\psi'|]) && (2.74)\\ &\overset{(b)}{\leq} S(\sum_k \mathrm{tr}_{SR}[P_k|\psi'\rangle\langle\psi'|P_k]) && (2.75)\\ &\overset{(c)}{=} S(\sum_k p_k\rho_k^{MB_M}) && (2.76)\\ &\overset{(d)}{\leq} H\{p_k\} + \sum_k p_k S(\rho_k^{MB_M}) && (2.77) \end{aligned}$$

where the equality (a) follows from $\mathrm{tr}_{MB_M}[|\psi'\rangle\langle\psi'|] = \rho'_{SR}$, the inequality (b) follows from the general formula $S(\rho) \leq S(\sum_l P_l\rho P_l)$, the equality (c) follows from the definition of $\rho_k^{MB_M}$, , and the inequality (d) follows from the general formula $S(\sum_l q_l\rho_l) \leq H\{q_l\} + \sum_l q_l S(\rho_l)$. □

Finally, we prove Lemma 2.

Proof of Lemma 2: Let us refer to the optimal ensemble of $\rho_{AA'}$ as $\{r_m, \left|\psi_m^{AA'}\right\rangle\}$; in other words, $E_F^{A-A'}(\rho_{AA'}) = \sum_m r_m E^{A-A'}(\left|\psi_m^{AA'}\right\rangle)$ holds. We also refer to $\mathrm{tr}_{A'}[\left|\psi_m^{AA'}\right\rangle\left\langle\psi_m^{AA'}\right|]$ as ρ_m^A. Note that (2.68) is equivalent to

$$S(\sum_m r_m\rho_m^A) \leq \sum_m r_m S(\rho_m^A) + S(\sum_m r_m \left|\psi_m^{AA'}\right\rangle\left\langle\psi_m^{AA'}\right|). \tag{2.78}$$

After straightforward algebra, we can reduce (2.78) into

$$\sum_m r_m D(\rho_m^A||\rho^A) \leq \sum_m r_m D(\left|\psi_m^{AA'}\right\rangle\left\langle\psi_m^{AA'}\right| ||\rho_{AA'}). \tag{2.79}$$

Because the relative entropy decreases after partial trace, the inequality (2.79) holds clearly. We have thereby completed the proof of Lemma 2. □

2.4 Achievability of the equality of the principle of maximal work

In the sections 2.1, 2.2 and 2.3, we derived several thermodynamical inequalities. However, there was neither a proof or a counterproof that the equalities of the inequalities are generally achievable. Tasaki's derivation of (2.4) does not tell us whether there exists a unitary U on SB which achieves the equality of (2.4). Under the assumption that there exists a unitary U on SB which achieves the equality of (2.4), Sagawa and Ueda give an example of the information isothermal process which achieves the equality of (2.16). Under the same assumption, Jacobs proved the achievability of the equality of (2.16) more generally [26]. However, these proofs assume that there exists a unitary on SB which achieves the equality of (2.4).

In 2014, Skrzypczyk, Short, and Popescu constructed a concrete setup of the fully quantum work extraction, and shown the second law and the achievability of the equality of the inequality $W_{\text{ext}} \leq -\Delta F$ [12]. In the present section, we review their results in Ref. [12].

2.4.1 Setup and the thermodynamical quantities

We consider the total system as a composit system of a thermodynamic system S, a heat bath B with inverse temperature β, and a work storage W. The system S is an arbitrary finite-dimensional system with an arbitrary Hamiltonian H_S. We define the thermodynamic quantities of the system S which is in the state ρ as follows; the internal energy $U(\rho) := \mathrm{Tr}[\rho H_S]$, the entropy $S(\rho) := -\mathrm{Tr}[\rho \log \rho]$, and the Helmholtz free energy $F(\rho) := U - \frac{1}{\beta}S$. Note that the definition of the free energy in the present section is different from that of the sections 2.1, 2.2 and 2.3; in the present section, the Helmholtz free energy is a function of the state ρ. We take an arbitrary fixed state ρ_S as the initial state of the system S. We consider the heat bath B as an unlimited source of supply of finite-dimensional systems $\{B_m\}_{m=1}^{\infty}$ with arbitrary Hamiltonians $\{H_{B_m}\}_{m=1}^{\infty}$. The initial states ρ_{B_m} of B_m are given by Gibbs states $\tau_{B_m} := \exp(-\beta H_{B_m})/Z(\beta, H_{B_m})$. When, the thermodynamical process turns the states of B_m into σ_{B_m}, we define the absorbed heat $Q := \sum_m \mathrm{Tr}[H_{B_m}(\tau_{B_m} - \sigma_{B_m})]$. The work storage W is a suspended weight with the Hamiltonian $H_W = mg\hat{x}$, where $\hat{x}$ is the position operator. We define the extracted work W_{ext} as the average energy gain of W; if the initial and the final state are ρ_W and σ_W, the extracted work is expressed as $W_{\text{ext}} = \mathrm{Tr}[H_W(\sigma_W - \rho_W)]$. We also define a translation operator Γ_a, which translates the position of the weight as $\Gamma_a|x\rangle = |x+a\rangle$, where $|x\rangle$ and $|x+a\rangle$ are the eigenstates of $\hat{x}$ whose eigenvalues are x and $x+a$.

2.4.2 Isothermal operation

Under the above setup, we consider a unitary transformation U of the composit system SBW as an isothermal operation. We request the following three constraints of U.

- The unitary transformation U conserves the average energy of SBW for the fixed initial states of S and B

but for an arbitrary initial state of W. Namely, the following equality holds;

$$\mathrm{Tr}[(H_S+\sum_m H_{B_m}+H_W)(\rho_S\otimes(\otimes_m\tau_{B_m})\otimes\rho_W)]=\mathrm{Tr}[(H_S+\sum_m H_{B_m}+H_W)U(\rho_S\otimes(\otimes_m\tau_{B_m})\otimes\rho_W)U^\dagger] \tag{2.80}$$

- The dynamics of the composit system SB does not depend on the initial state of W. Namely, the following equality holds for arbitrary ρ_W and ρ'_W;

$$\mathrm{Tr}_W[U(\rho_S\otimes(\otimes_m\tau_{B_m})\otimes\rho_W)U^\dagger]=\mathrm{Tr}_W[U(\rho_S\otimes(\otimes_m\tau_{B_m})\otimes\rho'_W)U^\dagger] \tag{2.81}$$

- The unitary U commutes with the translation operator Γ_a for an arbitrary real number a.

Because of the second constraint, the dynamics of SB must be unital, namely,

$$\mathrm{Tr}_W[U(\hat{1}_{SB}\otimes\rho_W)U^\dagger]=\hat{1}_{SB} \tag{2.82}$$

holds. (*Proof :* Because of the second constraint,

$$\mathrm{Tr}_W[U(\hat{1}_{SB}\otimes\rho_W)U^\dagger]=\mathrm{Tr}_W[U(\hat{1}_{SB}\otimes\hat{1}_{SB})U^\dagger] \tag{2.83}$$

holds. The right-hand side of (2.83) is clearly equal to $\hat{1}_{SB}$. □)

We refer to the final states of S, B and W as σ_S, σ_B and σ_W, where

$$\sigma_S := \mathrm{Tr}_{BW}[U(\rho_S\otimes(\otimes_m\tau_{B_m})\otimes\rho_W)U^\dagger] \tag{2.84}$$

$$\sigma_B := \mathrm{Tr}_{SW}[U(\rho_S\otimes(\otimes_m\tau_{B_m})\otimes\rho_W)U^\dagger] \tag{2.85}$$

$$\sigma_W := \mathrm{Tr}_{SB}[U(\rho_S\otimes(\otimes_m\tau_{B_m})\otimes\rho_W)U^\dagger] \tag{2.86}$$

2.4.3 The second law

Let us prove that we cannot obtain a positive quantity of W_{ext} without changing the state of the system S; $\rho_S=\sigma_S$[3] In the present subsection, we prove the second law by the different way from Ref. [12], as our proof is simpler. Because of $\rho_S=\sigma_S$ and because the unitary U conserves the total energy, we have to make Q positive in order to make W_{ext} positive; namely, we have to take an isothermal process which decreases the average energy of B. Because the Gibbs state is the maximal-entropy state with given average energy, an isothermal process which decreases the average energy of B also decreases the entropy of B. Thus, if we could obtain a positive quantity of W_{ext} without changing the state of the system S, there would exist an isothermal process which satisfies $S(\sigma_B)-S(\rho_B)=:\Delta S_B<0$ and $\rho_S=\sigma_S$.

Let us prove the above isothermal process does not exist. Because the dynamics of SB is unital, $\Delta S_{SB}\ge 0$ holds. Because the von Neumann entropy is subadditive and because of $\rho_S=\sigma_S$, the inequlaity $\Delta S_{SB}\ge 0$ reduces to $\Delta S_B\ge 0$. □

2.4.4 The achievability of the equality of the principle of maximal work

Finally, we construct an N-step isothermal process which changes the state of S from $\rho_S=\sum_n p_n|\psi_n\rangle\langle\psi_n|$ to $\sigma_S=\sum_n p'_n|\psi'_n\rangle\langle\psi'_n|$ and satisfies $W_{\mathrm{ext}}=F(\rho_S)-F(\sigma_S)-O(1/N)$. We construct each step of the process as a combination of a unitary transformation V_1 on SW and a unitary construction V_2 on SBW. The unitary V_1 is given as

$$V_1 := \sum_n |E_n\rangle\langle\psi_n| \otimes \Gamma_{\epsilon_n}, \tag{2.87}$$

where $\{|E_n\rangle\}$ are the energy eigenstates of the system S, and where $\epsilon_n := \langle\psi_n|H_S|\psi_n\rangle - E_n$. Note that the unitary V_1 conserves the entropy of S, the entropy of SW and the average of energy of SW. Thus, V_1 satisfies $W_{\text{ext}} = F(\rho_S) - F(\rho'_S)$, where $\rho'_S := \mathrm{Tr}_{BW}[V_1(\rho_S \otimes (\otimes_m \tau_{B_m}) \otimes \rho_W)V_1^\dagger]$.

The unitary V_2 turns the state $\sum_n p_n|E_n\rangle\langle E_n|$ into $\sum_n q_n|E_n\rangle\langle E_n|$. For simplicity, we treat only the case in which $q_0 = p_0 - \delta p$, $q_1 = p_1 + \delta p$ and $q_n = p_n$ for $n \geq 2$, as an example. As the initial state of a qubit B_m for the transformation V_2, we take the Hamiltonian of H_{B_m} whose Gibbs state satisfies

$$\tau_{B_m} = \frac{q_0}{q_0 + q_1}|0\rangle\langle 0| + \frac{q_1}{q_0 + q_1}|1\rangle\langle 1|. \tag{2.88}$$

We define the unitary V_2 as follows:

$$V_2|E_0\rangle_S|1\rangle_{B_m}|x\rangle_W := |E_1\rangle_S|0\rangle_{B_m}|x + \epsilon\rangle_W, \tag{2.89}$$

where $\epsilon := E_{B_m} - E_1 + E_0$ and E_{B_m} is the difference of eigenvalues of H_{B_m}. The extracted work W_{ext} in V_2 is equal to $\epsilon\delta p$. The change of the inner energy of S is equal to $\delta U = \delta p(E_1 - E_0)$. The change of the entropy of S is equal to $\delta S_S = \delta p \beta E_{B_m} + O(\delta p^2)$. Thus the change of the free energy is approximately equal to the extracted work; $W_{\text{ext}} = \delta F + O(\delta p)$.

Now, we can construct the isothermal process which changes the state of S from ρ_S to σ_S and satisfies $W_{\text{ext}} = F(\rho_S) - F(\sigma_S) - O(1/N)$. The unitary V_1 turns ρ_S into $\sum_n p_n|E_n\rangle\langle E_n|$. We can turn $\sum_n p_n|E_n\rangle\langle E_n|$ into $\sum_n p'_n|E_n\rangle\langle E_n|$ by using V_2 repetedly. Finally, the unitary $V_1'^\dagger$ turns $\sum_n p'_n|E_n\rangle\langle E_n|$ into $\sum_n p'_n|\psi'_n\rangle\langle\psi'_n|$, where we obtain V'_1 substituting $|\psi'_n\rangle$ for $|\psi_n\rangle$ of V_1. Note that V_1, V_2 and $V_1'^\dagger$ satisfy $W_{\text{ext}} = F(\rho_S) - F(\sigma_S)$ approximately. The isothermal process which consists of V_1, V_2 and $V_1'^\dagger$ satisfies $W_{\text{ext}} = F(\rho_S) - F(\sigma_S) - O(1/N)$.
□

Chapter 3

Work Extraction as a Measurement Process

3.1 A Contradiction between Two Scenarios for Work Extraction

As we reviewed in Chapter 2, there exist two well-known scenarios for the work extraction from quantum systems:

Semi-classical scenario [8–10, 25–30]: In this scenario, the classical external operator performs the unitary time evolution $U_I := T_{\rightarrow} \exp(\int -iH_I(t)dt)$ on I by time-dependently controlling the control parameter of the Hamiltonian $H_I(t)$ of the internal system I (which usually consists of the system S and the heat bath B). During the time evolution, the energy is transmitted from the internal sytem to the external controller through the back reaction of the control parameter, and we regard the energy loss as the extracted work [8, Section 2].

Fully quantum scenario [11, 12, 31, 33–37] In this scenario, we consider not only the internal system I but also the external system E_X, whose Hilbert spaces are $\mathcal{H}_I$ and $\mathcal{H}_{E_X}$, respectively. We perform an arbitrary unitary transformation U_{IE_X} on the total system IE_X which conserves the energy of the total system IE_X, and regard the energy gain of E_X 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_X} and an arbitrary fixed initial state ρ_{E_X} of the external system E_X, the true time evolution of the internal system I is given by

$$\Lambda_I(\rho_I) = \mathrm{Tr}_{E_X}[U_{IE_X}\rho_I \otimes \rho_{E_X} U^{\dagger}_{IE_X}], \tag{3.1}$$

where ρ_I is an arbitrary initial state of the internal system. According to the semi-classical senario, the time evolution of the internal sytsem is the unitary U_I. In order to $\Lambda_I(\rho_I) = U_I\rho_I U_I^{\dagger}$, the unitary U_{IE_X} should be written as $U_I \otimes V_{E_X}$, where V_{E_X} is a unitary transformation on E_X. However, such a unitary does not cause the energy transfer between I and E_X, because $U_I \otimes V_{E_X}$ means that I and E_X 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 ρ_I. If E_X is large enough, there might be a special Hamiltonian H_{E_X} of E_X, a special initial state ρ_{E_X} of E_X and a special unitary operation V_{IE_X} on IE_X 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 the set $\{V_{IE_X}, \rho_{E_X}, H_{E_X}\}$ 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_X for an arbitrary initial state of I.

The above explanation sounds persuasive. However, we pose two questions still exist about the explanation;

Question 1: Does the set $\{V_{IE_X}, \rho_{E_X}, H_{E_X}\}$ really exist?

Question 2: Can we know the amount of the extracted work from observing E_X?

The answer to Question 1 is Yes. In the next subsection 3.1.1, we give an example of the set $\{V_{IE_X}, \rho_{E_X}, H_{E_X}\}$. However, the answer to Question 2 is No. We will show in Subsection 3.1.2 that, whenever Λ_I is approximately a unitary transformation, we can know practically nothing about the amount of the extracted work from observing E_X. Note that in the classical work extraction, the answer to Question 2 is clearly Yes. For example, we can know the amount of the extracted work by seeing the change in the position of a suspended weight. In the quantum work extraction, the situation is quite different. In Subsection 3.1.2, we will show a trade-off inequality, which tells us that in order to know the amount of the extracted energy, we have to destroy the coherence of the internal system; namely, the work extraction must be a measurement.

3.1.1 The answer to Question 1: an example of the set $\{V_{IE_X}, \rho_{E_X}, H_{E_X}\}$

Let us give an example of the set $\{V_{IE_X}, \rho_{E_X}, H_{E_X}\}$ which satisfies

$$[V_{IE_X}, H_I + H_{E_X}] = 0, \tag{3.2}$$

$$\Lambda_I(\rho_I) \approx U_I\rho_I U_I^\dagger, \text{ for any } \rho_I. \tag{3.3}$$

In order to make (3.3) more specific mathematically, we define the degree of approximation ϵ between Λ_I and the unitary transformation U_I on $\mathcal{H}_I$ as follows:

$$b(\Lambda_I(\rho), U_I\rho U_I^\dagger) \le \epsilon \text{ for any } \rho, \tag{3.4}$$

where b is the Bures distance $b(\rho,\sigma) := \sqrt{1 - F(\rho,\sigma)}$ with F being the fidelity $F(\rho,\sigma) := \mathrm{Tr}[\sqrt{\sqrt{\sigma}\rho\sqrt{\sigma}}]$.

For simplicity, let us consider an example of $\{V_{IE_X}, \rho_{E_X}, H_{E_X}\}$

$$H_I = \sum_{j=1}^{D} j|j\rangle_I\langle j|_I, \tag{3.5}$$

where D is the dimensionality of $\mathcal{H}_I$. (We can treat the more general examples in the same way.) For an arbitrary unitary transformation $U_I := \sum_{k,l} u_{kl}|k\rangle_I\langle l|_I$, we can take the set $\{V_{IE_X}, \rho_{E_X}, H_{E_X}\}$ as follows:

$$V_{IE_X}|k\rangle_I|m\rangle_{E_X} := \sum_{l=1}^{D} u_{kl}|l\rangle_I|m+k-l\rangle_{E_X} \tag{3.6}$$

$$\rho_{E_X} = |\psi\rangle\langle\psi| \text{ with } |\psi\rangle := \sum_{m=1}^{4D\lceil 1/\epsilon^2\rceil} \frac{1}{\sqrt{4D\lceil 1/\epsilon^2\rceil}}|m\rangle, \tag{3.7}$$

$$H_{E_X} := \sum_{k=-\infty}^{\infty} k|k\rangle_{E_X}\langle k|, \tag{3.8}$$

where $\lceil x\rceil$ is the ceiling function of x.

Proof: Because the unitary V_{IE_X} turns the energy pure eigenstate $|k\rangle_I|m\rangle_{E_X}$ of $H_I + H_{E_X}$ into another energy pure eigenstate of $H_I + H_{E_X}$ whose eigenvalue is $k+m$ for arbitrary k and m, the unitary V_{IE_X} clearly satisfies (3.2). Thus, we only have to show that the set $\{V_{IE_X}, \rho_{E_X}, H_{E_X}\}$ satisfies (3.4) for an arbitrary pure state $|\phi_I\rangle := \sum_{i=1}^{D} a_i\,|i\rangle_I$ of the internal system. By writing $|\psi\rangle$ as $\sum_{k=-\infty}^{\infty} C_k|k\rangle$, we obtain

$$V_{IE_X}|\phi\rangle_I|\psi\rangle = V_{IE_X}\sum_{i=1}^{D}\sum_{k=-\infty}^{\infty} a_i C_k\,|i\rangle_I\,|k\rangle_{E_X} \tag{3.9}$$

$$= \sum_i\sum_j\sum_k u_{ij}a_iC_k\,|j\rangle_I\,|k+i-j\rangle_{E_X} \tag{3.10}$$

$$= \sum_i\sum_j\sum_k u_{ij}a_iC_{k-i+j}\,|j\rangle_I\,|k\rangle_{E_X}\,. \tag{3.11}$$

In order to derive $b(\Lambda_I(|\phi\rangle_I\langle\phi|_I), U_I|\phi\rangle_I\langle\phi|_IU_I^\dagger) < \epsilon$, we derive an inequality about $F(\Lambda_I(|\phi\rangle_I\langle\phi|_I), U_I|\phi\rangle_I\langle\phi|_IU_I^\dagger)$. Because of (3.11), we obtain

$$F(\Lambda_I(|\phi\rangle_I\langle\phi|_I), U_I|\phi\rangle_I\langle\phi|_IU_I^\dagger) = \langle\phi|_IU_I^\dagger\Lambda_I(|\phi\rangle_I\langle\phi|_I)U_I|\phi\rangle_I \tag{3.12}$$

$$= \sum_k\langle\phi|_I\langle k|_{E_X}U_I^\dagger(V_{IE_X}|\phi\rangle_I|\psi\rangle\langle\phi|_I\langle\psi|V_{IE_X}^\dagger)U_I|\phi\rangle_I|k\rangle_{E_X} \tag{3.13}$$

$$= \sum_{i,i',i'',i''',j,j',k} u^*_{i''',j}u_{i'',j}a_{i''}a^*_{i'''}C_{k-i''+j'}C_{k-i+j} \tag{3.14}$$

Because of the definition of $|\psi\rangle$, the equalities $C_k = C_{k-i+j} = 1/\sqrt{4D\lceil 1/\epsilon^2\rceil}$ hold for the range $D+1 \le k \le$

$D(4\lceil 1/\epsilon^2\rceil - 1)$. Thus, we obtain

$$\begin{aligned}
&\sum_{i,i',i'',i''',j,j',k} u^*_{i''',j} u_{i'',j} a_{i''} a^*_{i'''} C_{k-i''+j'} C_{k-i+j} \\
&= \sum_{k=D+1}^{D(4\lceil 1/\epsilon^2\rceil - 1)} \sum_{i,i',i'',i''',j,j'} u^*_{i''',j} u_{i'',j} a_{i''} a^*_{i'''} C_{k-i''+j'} C_{k-i+j} + \sum_{\text{other } k} \sum_{i,i',i'',i''',j,j'} u^*_{i''',j} u_{i'',j} a_{i''} a^*_{i'''} C_{k-i''+j'} C_{k-i+j} \\
&= \sum_{k=D+1}^{D(4\lceil 1/\epsilon^2\rceil - 1)} \sum_{i,i',i'',i''',j,j'} u^*_{i''',j} u_{i'',j} a_{i''} a^*_{i'''} \frac{1}{4D\lceil 1/\epsilon^2\rceil} + \sum_{\text{other } k} \sum_{i,i',i'',i''',j,j'} u^*_{i''',j} u_{i'',j} a_{i''} a^*_{i'''} C_{k-i''+j'} C_{k-i+j} \\
&= \sum_{i,i',i'',i''',j,j'} u^*_{i''',j} u_{i'',j} a_{i''} a^*_{i'''} \frac{D(4\lceil 1/\epsilon^2\rceil - 2)}{4D\lceil 1/\epsilon^2\rceil} + \sum_{\text{other } k} \sum_{i,i',i'',i''',j,j'} u^*_{i''',j} u_{i'',j} a_{i''} a^*_{i'''} C_{k-i''+j'} C_{k-i+j} \\
&= \frac{D(4\lceil 1/\epsilon^2\rceil - 2)}{4D\lceil 1/\epsilon^2\rceil} - \left| \sum_{\text{other } k} \sum_{i,i',i'',i''',j,j'} u^*_{i''',j} u_{i'',j} a_{i''} a^*_{i'''} C_{k-i''+j'} C_{k-i+j} \right| \\
&\geq \frac{D(4\lceil 1/\epsilon^2\rceil - 2)}{4D\lceil 1/\epsilon^2\rceil} - \frac{2D}{4D\lceil 1/\epsilon^2\rceil} = \frac{\lceil 1/\epsilon^2\rceil - 1}{\lceil 1/\epsilon^2\rceil} \geq 1 - \epsilon^2
\end{aligned} \tag{3.15}$$

Namely, we obtain

$$F(\Lambda_I(|\phi\rangle_I\langle\phi|_I), U_I|\phi\rangle_I\langle\phi|_I U_I^\dagger) \geq 1 - \epsilon^2. \tag{3.16}$$

By substituting the left-hand side of (3.16) for the definition of the Bures distance, we obtain

$$b(\Lambda_I(|\phi\rangle_I\langle\phi|_I), U_I|\phi\rangle_I\langle\phi|_I U_I^\dagger) \leq \sqrt{1 - \sqrt{1-\epsilon^2}} \leq \epsilon \tag{3.17}$$

Therefore, (3.4) is satisfied. □

The above example gives not only the answer to Question 1, but also a good insight into Question 2. Note that the state $|\psi\rangle_{E_X}$ is very broad in the energy space. If we take an initial state of E_X whose support is narrow in the energy space, the inequality (3.4) does not hold. However, the states which are broad in the energy space, changes little under the unitary V_{IE_X} for an arbitrary initial state of I. This fact leads us to the following anticipation; whenever the unitary U_{IE_X} satisfies (3.3), the final state of E_X is hardly affected by the initial state of I. In the next subsection 3.1.2, we will show that the anticipation is right, by applying the knowledge about the relationship between the information gain and the coherence destruction to the work extraction.

3.1.2 The answer to Question 2: the trade-off relation

Theorem 1. *When the unitary transformation U_{IE_X} and the initial state ρ_{E_X} satisfy*

$$b(\Lambda_I(\rho), U_I\rho U_I^\dagger) \leq \epsilon \text{ for any } \rho \tag{3.18}$$

for a unitary U_I*, then the following inequality holds for arbitrary states* ρ *and* ρ' *on* $\mathcal{H}_I$ [4] *:*

$$b(\sigma^{\rho}_{E_X}, \sigma^{\rho'}_{E_X}) \leq 4\sqrt{\epsilon}, \tag{3.19}$$

where $\sigma^{\rho}_{E_X} := \mathrm{Tr}_I[U_{IE_X}\rho \otimes \rho_{E_X} U^{\dagger}_{IE_X}]$.

Proof : The Bures distance satisfies the following properties [58]:

$$\begin{aligned}
b(\rho_1, \rho_3) &\leq b(\rho_1, \rho_2) + b(\rho_2, \rho_3), && (3.20)\\
b(\rho, \rho') &= b(U\rho U^{\dagger}, U\rho' U^{\dagger}), && (3.21)\\
b(\rho, \rho') &\geq b(\kappa(\rho), \kappa(\rho')), && (3.22)\\
b^2(\rho \otimes \sigma, \rho' \otimes \sigma') &= b^2(\rho, \rho') + b^2(\sigma, \sigma') - b^2(\rho, \rho') b^2(\sigma, \sigma'), && (3.23)\\
b\Big(\frac{\rho + \rho'}{2}, \rho'\Big) &\leq \sqrt{1 - \frac{1}{\sqrt{2}}}, && (3.24)
\end{aligned}$$

where κ is an arbitrary CP-TP map.

We carry out the proof (3.19) in cases of $b(\rho_I, \rho'_I) \leq 2\epsilon$, $2\epsilon \leq b(\rho_I, \rho'_I) \leq \sqrt{1 - \sqrt{1/2}}$, and $\sqrt{1 - \sqrt{1/2}} \leq b(\rho_I, \rho'_I) \leq 1$. In the case of $b(\rho_I, \rho'_I) \leq 2\epsilon$, we can derive (3.19) as follows:

$$\begin{aligned}
4\sqrt{\epsilon} \geq 2\epsilon \geq b(\rho_I, \rho'_I) &\overset{(a)}{=} b(\rho_I \otimes \rho_{E_X}, \rho'_I \otimes \rho_{E_X})\\
&\overset{(b)}{=} b(\sigma^{\rho_I}_{IE_X}, \sigma^{\rho'_I}_{IE_X}) \overset{(c)}{\geq} b(\sigma^{\rho_I}_{E_X}, \sigma^{\rho'_I}_{E_X}). && (3.25)
\end{aligned}$$

where (a) follows from (3.23), (b) follows from (3.21), and (c) follows from (3.22) whose κ is the partial trace of I.

Next, we prove (3.19) in the case of $2\epsilon \leq b(\rho_I, \rho'_I) \leq \sqrt{1 - \sqrt{1/2}}$. Because of (3.18), (3.20) and (3.21), we obtain

$$\begin{aligned}
b(\Lambda_I(\rho_I), \Lambda_I(\rho'_I)) &\geq b(U_I\rho_I U_I^{\dagger}, U_I\rho'_I U_I^{\dagger}) - b(\Lambda_I(\rho_I), U_I\rho_I U_I^{\dagger}) - b(\Lambda_I(\rho'_I), U_I\rho'_I U_I^{\dagger}) && (3.26)\\
&\geq b(\rho_I, \rho'_I) - 2\epsilon. && (3.27)
\end{aligned}$$

From (3.22) and (3.23), we also obtain

$$\begin{aligned}
&b(\sigma^{\rho_I}_{IE_X}, \sigma^{\rho'_I}_{IE_X}) \geq b(\Lambda_I(\rho_I) \otimes \sigma^{\rho_I}_{E_X}, \Lambda_I(\rho'_I) \otimes \sigma^{\rho'_I}_{E_X})\\
&= \sqrt{b^2(\Lambda_I(\rho_I), \Lambda_I(\rho'_I)) + b^2(\sigma^{\rho_I}_{E_X}, \sigma^{\rho'_I}_{E_X}) - b^2(\Lambda_I(\rho_I), \Lambda_I(\rho'_I)) b^2(\sigma^{\rho_I}_{E_X}, \sigma^{\rho'_I}_{E_X})}. && (3.28)
\end{aligned}$$

Moreover, because of (3.21) and (3.23),

$$b(\sigma^{\rho_I}_{IE_X}, \sigma^{\rho'_I}_{IE_X}) = b(\rho_I \otimes \rho_{E_X}, \rho'_I \otimes \rho_{E_X}) = b(\rho_I, \rho'_I) \tag{3.29}$$

[4]Here, we use the Bures distance in order to define the approximation degree between the time evolution Λ_I of I and the unitary transformation U_I. As in Refs. [48] and [49], we can give a similar trade-off relation between the information gain of E_X and the disturbance of I, which is defined with using the coherent information. We use the Bures distance because the Bures distance enables us to make the scope of application of Theorem 1 larger than the coherent information. For example, we can construct the set of a special initial state ρ_{E_X} of E_X and a unitary interaction U_{IE_X} on IE_X which satisfies (3.18) for an arbitrary ρ_I, but the disturbance of the internal system is large for a specific ρ_I^{spec}.

holds. Thus, substituting (3.27) and (3.29) for (3.28), we obtain

$$4\epsilon\frac{b(\rho_I,\rho'_I)-\epsilon}{1-(b(\rho_I,\rho'_I)-2\epsilon)^2}\geq b^2(\sigma^{\rho_I}_{E_X},\sigma^{\rho'_I}_{E_X}). \tag{3.30}$$

Note that

$$1\geq\frac{b(\rho_I,\rho'_I)-\epsilon}{1-(b(\rho_I,\rho'_I)-2\epsilon)^2}$$

holds for the case of $2\epsilon\leq b(\rho_I,\rho'_I)\leq\sqrt{1-\sqrt{1/2}}$. Therefore, (3.19) holds for the case of $2\epsilon\leq b(\rho_I,\rho'_I)\leq\sqrt{1-\sqrt{1/2}}$.

Finally, we prove (3.19) in the case of $\sqrt{1-\sqrt{1/2}}\leq b(\rho_I,\rho'_I)\leq 1$. Note that $b(\rho_I,\frac{\rho_I+\rho'_I}{2})\leq\sqrt{1-\sqrt{1/2}}$ and $b(\rho'_I,\frac{\rho_I+\rho'_I}{2})\leq\sqrt{1-\sqrt{1/2}}$ hold for arbitrary ρ_I and ρ'_I. Therefore, we obtain

$$b(\sigma^{\frac{\rho_I+\rho'_I}{2}}_{E_X},\sigma^{\rho'_I}_{E_X})\leq 2\sqrt{\epsilon}, \tag{3.31}$$

$$b(\sigma^{\frac{\rho_I+\rho'_I}{2}}_{E_X},\sigma^{\rho_I}_{E_X})\leq 2\sqrt{\epsilon}. \tag{3.32}$$

Hence, we obtain (3.19) from (3.20):

$$b(\sigma^{\rho_I}_{E_X},\sigma^{\rho'_I}_{E_X})\leq 2\sqrt{\epsilon}+2\sqrt{\epsilon}=4\sqrt{\epsilon}. \tag{3.33}$$

□

The inequality (3.19) implies that if we perform an approximate unitary time evolution on I, we cannot know the amount of the energy gain of E_X by observing E_X. The Bures distance $b(\rho,\sigma)$ is equal to the maximum of the Helinger distance $b_{\mathrm{c}}(\{p_m\},\{q_m\})$ [58]:

$$b(\rho,\sigma)=\max_{\{E_m\}:\mathrm{POVM}}b_{\mathrm{c}}(\{p_m\},\{q_m\}), \tag{3.34}$$

where $p_m:=\mathrm{Tr}[\rho E_m]$ and $q_m:=\mathrm{Tr}[\sigma E_m]$. That is, the Bures distance $b(\rho,\sigma)$ expresses the limit of the distinguishability between ρ and σ under the POVM measurements. Thus, if we perform an approximate unitary time evolution on I, the observation on E_X cannot distinguish the final states of E_X even though I starts from different initial states. This fact also implies that the energy transfer from I to E_X is the heat rather than the work when the time evolution of I is approximately unitary, because we have to guess the amount of the energy transfer from observing I. Thus, the unitary semi-classical scenario is inappropriate as the work extraction scenario.

In order to avoid the above problem, we have to take a large value of ϵ. This fact shows that in order to know the amount of the extracted energy, we have to destroy the coherence of I; namely, a work extraction must be a measurement.

3.2 Work extraction as a measurement process

Based on the previous section, let us formulate the work extraction as a measurement process in the present section. Here, we show a rough sketch of the formulation. As the previous section, we consider the total system IE_X which consists of the internal system I and the external system E_X. The internal system I consists of the system S and the heat baths $\{B_m\}$, and the external system E_X contains the work storage W. When we consider the work extraction with feedback control E_X consists of the work storage W and the memory system M. When we consider the work extraction with feedback control E_X is just the work storage W. We perform a unitary transformation on IE_X which conserves the total energy of IE_X. After the unitary transformation, we perform a measurement on E_X. We define the work extraction as the energy transfer from I to E_X during the above process, which satisfies the following conditions:

Condition 1 We can know the amount of the amount of the energy loss of I from the outcome of the measurement on E_X.

Condition 2 The entropy of the work storage W does not increase during the unitary transformation on IE_X.

Note that the time evolution of the internal system is a measurement process. In the present section, we show the detail of the above rough sketch.

3.2.1 CP-work extraction

We firstly focus on the time evolution of the internal system I of the work extraction in the present subsection. As the minimal requirement, we demand that the time evolution is a measurement on I such that the average of the measured values of the measurement is equal to the average energy loss of I during the measurement;

Definition 1 (CP-work extraction). *Let us take an arbitrary set of a CP-instrument $\{\mathcal{E}_j\}_{j\in J}$ and measured values $\{w_j\}_{j\in J}$, where each $\mathcal{E}_j$ is a completely positive map, and where $\sum_j \mathcal{E}_j$ is a completely positive and trace preserving (CPTP) map, and where J is the set of the outcome, which can be either a discrete set or a continuous set. When the set $\{\mathcal{E}_j, w_j\}_{j\in J}$ satisfy the following equality for any state ρ on $\mathcal{H}_I$, we refer to the set $\{\mathcal{E}_j, w_j\}_{j\in J}$ as the CP-work extraction:*

$$\mathrm{Tr}H_I\rho = \sum_j w_j \mathrm{Tr}\mathcal{E}_j(\rho) + \sum_j \mathrm{Tr}H_I\mathcal{E}_j(\rho), \tag{3.35}$$

where H_I is the Hamiltonian of I.

There are two important points in the above definition. First, we does not any request for what $\{\mathcal{E}_j\}$ measures. Thus, $\{\mathcal{E}_j\}$ might not be the measurement about energy. For example, we can measure some particle's track as $\{\mathcal{E}_j\}$. In that case, $\{w_j\}$ is given as a function of the track, and we can take an arbitrary function $\{w_j\}$ which satisfies (3.35).

Second, whereas H_I does not change during the CP-work extraction, we can treat by the method in Ref. [33] the case in which the Hamiltonians of the working body and the heat baths changes do. To do so, we divide the internal system I into two subsystems I_1 and I_2. The first part I_1 consists of the working body and the heat baths, while the second part I_2 controls the Hamiltonian of I_1. Let the total Hamiltonian of I be

$$H_I = \sum_\lambda H_\lambda \otimes |\lambda\rangle\langle\lambda|, \tag{3.36}$$

where H_λ is the Hamiltonian of I_1 and where $\{|\lambda\rangle\}$ is a orthonomal basis of I_2. The CP-work extraction on I in which the state of I changes from $\rho_{I_1} \otimes |\lambda_{\rm ini}\rangle\langle\lambda_{\rm ini}|$ to $\sigma_{I_1} \otimes |\lambda_{\rm fin}\rangle\langle\lambda_{\rm fin}|$ corresponds to the thermodynamic operation of I_1 in which the Hamiltonian and the state of I_1 change from $(H_{\lambda_{\rm ini}}, \rho_{I_1})$ to $(H_{\lambda_{\rm fin}}, \sigma_{I_1})$.

Now we have formulated of the work extraction for the internal system with the minimal request. However, it is too general for practical purpose. More specifically, the average $\sum_j w_j {\rm Tr}\mathcal{E}_j(\rho)$ is the averaged extracted work, but each value w_j may not be the extracted work in the case that the measurement outcome is j. Moreover, the CP-work extraction includes both of the work extractions with and without feedback control. Thus, we give two classes of the practical work extractions. The first class is called as the CP-strong work extraction, in which each value w_j means that the amount of the extracted work from I in the case that the measurement outcome is j.

Definition 2 (CP-strong work extraction). *Let us take an arbitrary set of a CP-instrument $\{\mathcal{E}_j\}_{j\in J}$ and measured values $\{w_j\}_{j\in J}$. Let $|x\rangle \in \mathcal{H}_I$ be an arbitrary normalized eigenvector of H_I with an eigenvalue h_x. We denote the spectral decomposition of H_I as $H_I = \sum_h hP_h$, where P_h is the projection to the energy eigenspace of H_I whose eigenvalue is h. When the following equality holds for each j, we refer to the set $\{\mathcal{E}_j, w_j\}_{j\in J}$ as the CP-strong work extraction.*

$$P_h\mathcal{E}_j(|x\rangle\langle x|)P_h \begin{cases} = \mathcal{E}_j(|x\rangle\langle x|) & (h = h_x - w_j), \\ = 0 & (otherwise). \end{cases} \tag{3.37}$$

The equations (3.37) means that if the initial state of the internal system I has the energy of a definitive value, then the internal system also has the energy of a definitive value, after j is determined, and the value w_j expresses the difference of energy between initial and final. Thus, when the initial state ρ_I of I is the diagonalized by $\{P_{I|y}\}$, the value w_j is equal to the average energy loss of I in the case the the measurement outcome is j. In this sense, each value w_j expresses the amount of the extracted work. As we show at the end of the present subsection, the CP-strong work extraction is the special case of the CP-work extraction.

Lemma 3. *When a set of $\{\mathcal{E}_j, w_j\}_{j\in J}$ is a CP-strong work extraction, it is also a CP-work extraction.*

The second class is called as the CP-unital work extraction, which corresponds to the work extraction without feedback control.

Definition 3 (CP-unital work extraction). *Let us take a CP-work extraction $\{\mathcal{E}_j, w_j\}_{j\in J}$. When the CPTP-map $\sum_j \mathcal{E}_j$ is unital, namely the equation $\sum_j \mathcal{E}_j(\hat{1}_I) = \hat{1}_I$ holds, we refer to the CP-work extraction $\{\mathcal{E}_j, w_j\}_{j\in J}$ as the CP-unital work extraction.*

Let us show that the work extraction without feedback control must be the CP-unital work extraction. Let the initial states of I and E_X be ρ_I and ρ_{E_X}. We perform a unitary transformation U_{IE_X} on IE_X, and perform a measurement $\{M_k\}$ on E_X. After the unitary transformation U_{IE_X}, the states of I and E_X become $\sum_j \mathcal{E}_j(\rho_I) = {\rm Tr}_{E_X}[U_{IE_X}(\rho_I \otimes \rho_{E_X})U_{IE_X}^\dagger]$ and $\Lambda(\sigma_{E_X}) := {\rm Tr}_I[U_{IE_X}(\rho_I \otimes \rho_{E_X})U_{IE_X}^\dagger]$ In the case of the work extraction without feedback, the external system E_X is just the work storage W. Thus, during the unitary U_{IE_X}, the entropy of the external system E_X does not increase;$S(\Lambda(\rho_{E_X})) = S(\rho_{E_X})$. Because the unitary transformation conserves the entropy, and because of the subadditibity of the entropy, we obtain

$$S(\rho_I)+S(\rho_{E_X})=S(\rho_I\otimes\rho_{E_X}) \;=\; S(U_{IE_X}\rho_I\otimes\rho_{E_X}U_{IE_X}^\dagger)\le S(\Lambda(\rho_{E_X}))+S(\sum_j\mathcal{E}_j(\rho_I)). \tag{3.38}$$

$$S(\rho_I) \;\le\; S(\sum_j\mathcal{E}_j(\rho_I)). \tag{3.39}$$

Because a unital CPTP-map conserves or increases the von Neumann entropy [61], the CP-unital work extraction satisfies (3.39). Because (3.39) holds for an arbitrary ρ_I,

$$S(\hat{1}/d)\le S(\sum_j\mathcal{E}_j(\hat{1}/d)) \tag{3.40}$$

holds, where d is the dimension of the internal system I. Because $S(\rho)<S(\hat{1}/d)$ holds for arbitrary $\rho\neq\hat{1}/d$, when (3.39) holds, $\sum_j\mathcal{E}_j(\hat{1}/d)=\hat{1}/d$ also holds. Thus, the time evolution of the internal system of the work extraction without feedback control must be unital.

Proof of Lemma 3: We only have to prove that $\{\mathcal{E}_j,w_j\}_{j\in J}$ satisfies (3.35). We denote the special decomposition of H_I as $H_I=\sum_h hP_h$, where P_h is the projection to the energy eigenspace of H_I whose eigenvalue is h. Let $\{|x\rangle\}$ be the energy eigenbasis of H_I, and $\{M_{j,k}\}$ be a set of operation elements for $\{\mathcal{E}_j\}$; namely,

$$\mathcal{E}_j(\rho)=\sum_k M_{j,k}\rho M_{j,k}^\dagger \tag{3.41}$$

holds for an arbitrary state ρ. Because of (3.37), the following equality holds for the matrix elements $m_{j,k}^{x',x}:=\langle x'|M_{j,k}|x\rangle$;

$$m_{j,k}^{x',x}=m_{j,k}^{x',x}\delta_{h_x-h_{x'},w_j} \tag{3.42}$$

where h_x and $h_{x'}$ is the energy eigenvalues of $|x\rangle$ and $|x'\rangle$. From (3.41), (3.42) and $\sum_{j,k}M_{j,k}^\dagger M_{j,k}=\hat{1}_I$, we obtain (3.35) as follows;

$$
\begin{aligned}
\sum_j \mathrm{Tr}[H_I \mathcal{E}_j(\rho)] &= \sum_j \sum_y \langle y|H_I \mathcal{E}_j(\rho)|y\rangle && (3.43)\\
&\stackrel{(a)}{=} \sum_{j,k} \sum_y \langle y|H_I M_{j,k}\rho M_{j,m}^\dagger|y\rangle && (3.44)\\
&= \sum_{j,k} \sum_y h_y \langle y|M_{j,k}\rho M_{j,k}^\dagger|y\rangle && (3.45)\\
&= \sum_{j,k} \sum_y \sum_{x,x'} h_y m_{j,k}^{y,x} r_{x,x'} (m_{j,k}^{y,x'})^* && (3.46)\\
&\stackrel{(b)}{=} \sum_{j,k} \sum_y \sum_{x,x'} h_y m_{j,k}^{y,x} r_{x,x'} (m_{j,k}^{y,x'})^* \delta_{h_x - h_y, w_j} \delta_{h_{x'} - h_y, w_j} && (3.47)\\
&= \sum_{j,k} \sum_y \sum_{x,x'} (h_x - w_j) m_{j,k}^{y,x} r_{x,x'} (m_{j,k}^{y,x'})^* \delta_{h_x, h_{x'}} && (3.48)\\
&= \sum_{j,k} \sum_y \sum_{x,x'} h_x m_{j,k}^{y,x} r_{x,x'} (m_{j,k}^{y,x'})^* \delta_{h_x, h_{x'}} - \sum_{j,k} \sum_y \sum_{x,x'} w_j m_{j,k}^{y,x} r_{x,x'} (m_{j,k}^{y,x'})^* \delta_{h_x, h_{x'}} && (3.49)\\
&\stackrel{(c)}{=} \sum_{x,x'} h_x r_{x,x'} \delta_{x,x'} \delta_{h_x, h_{x'}} - \sum_{j,k} \sum_y \sum_{x,x'} w_j m_{j,k}^{y,x} r_{x,x'} (m_{j,k}^{y,x'})^* \delta_{h_x, h_{x'}} && (3.50)\\
&= \mathrm{Tr}[H_I \rho] - \sum_{j,k} \sum_y \sum_{x,x'} w_j m_{j,k}^{y,x} r_{x,x'} (m_{j,k}^{y,x'})^* \delta_{h_x, h_{x'}} && (3.51)\\
&\stackrel{(d)}{=} \mathrm{Tr}[H_I \rho] - \sum_{j,k} \sum_y \sum_{x,x'} w_j m_{j,k}^{y,x} r_{x,x'} (m_{j,k}^{y,x'})^* \delta_{h_x, h_{x'}} \delta_{h_x - h_y, w_j} \delta_{h_{x'} - h_y, w_j} && (3.52)\\
&= \mathrm{Tr}[H_I \rho] - \sum_{j,k} \sum_y \sum_{x,x'} w_j m_{j,k}^{y,x} r_{x,x'} (m_{j,k}^{y,x'})^* \delta_{h_x - h_y, w_j} \delta_{h_{x'} - h_y, w_j} && (3.53)\\
&\stackrel{(e)}{=} \mathrm{Tr}[H_I \rho] - \sum_{j,k} \sum_y \sum_{x,x'} w_j m_{j,k}^{y,x} r_{x,x'} (m_{j,k}^{y,x'})^* && (3.54)\\
&= \mathrm{Tr}[H_I \rho] - \sum_j w_j \mathrm{Tr}[\mathcal{E}_j(\rho)] && (3.55)
\end{aligned}
$$

where the equality (a) follows from (3.41), the matrix elements $r_{x,x'}$ are defined as $r_{x,x'} := \langle x|\rho|x'\rangle$, the equality (b) follows from (3.42), the equality (c) follows from $\sum_{j,k} M_{j,k}^\dagger M_{j,k} = \hat{1}_I$, and the equalities (d) and (e) follow from (3.42). □

In the present subsection, we have defined the CP-work extraction as the measurement such that $\sum_j p_j w_j$ means the average work. We also have defined two classes of the CP-work extraction for practical use. The first one is the CP-strong work extraction, in which each value w_j means the extracted work in the case that the measurement outcome is j. The second one is the CP-unital work extraction, which corresponds to the work extractions without feedback control. For convenience of description, we refer to the CP-work extraction which is strong and unital at the same time as the CPSU-work extraction. Because the CPSU-work extraction is the work extraction without feedback control whose w_j means the amount of the extracted work, it is reasonable to consider all natural thermodynamical work extractions to be the CPSU-work extraction.

3.2.2 FQ-work extraction

In the previous subsection 3.2.1, we have focused on the internal system, and defined the CP-work extraction. In the present subsection, we consider the dynamics of the total system IE_X which realizes the CP-work extraction as the time evolution of the internal system I. As the minimal requirement, we demand that the time evolution of the total system IE_X conserves the average of energy of total system;

Definition 4 (Fully quantum (FQ) work extraction)**.** *Let us consider an external system $\mathcal{H}_{E_X}$ with the Hamiltonian H_{E_X}. If the unitary transformation U on $\mathcal{H}_I \otimes \mathcal{H}_{E_X}$ and the initial state ρ_{E_X} on $\mathcal{H}_{E_X}$ satisfy the following equation for any state ρ on $\mathcal{H}_I$, we refer to the set $(\mathcal{H}_{E_X}, H_{E_X}, \rho_{E_X}, U)$ as the FQ work extraction:*

$$\mathrm{Tr}H_I\rho + \mathrm{Tr}H_{E_X}\rho_{E_X} = \mathrm{Tr}(H_I + H_{E_X})U(\rho \otimes \rho_{E_X})U^\dagger. \tag{3.56}$$

We can reduce the FQ work extraction easily to the CP-work extraction (3.35) as follows. Let us denote the spectral decomposition of H_{E_X} by $H_{E_X} = \sum_j h_{E|j} P_{E|j}$, where $P_{E|j}$ is the projection to the energy eigenspace of H_{E_X} whose eigenvalue is $h_{E|j}$. We also define the CP map $\mathcal{E}_j$ on $\mathcal{H}_I$ as $\mathcal{E}_j(\rho) := \mathrm{Tr}_E[U(\rho \otimes \rho_{E_X})U^\dagger P_{E|j}]$. Finally, we define the measured value w_j as $w_j := h_{E|j} - \mathrm{Tr}H_{E_X}\rho_{E_X}$. We thereby obtain the CP-work extraction corresponding to the FQ work extraction. Hereafter, we refer to the above mapping from the FQ-work extraction to the CP-work extraction as FQ-CP map. We also refer to the CP-work extraction as $\{\mathcal{E}_j, w_j\}_{(\mathcal{H}_{E_X}, H_{E_X}, \rho_{E_X}, U)}$ when the FQ-CP map reduces the FQ work extraction $(\mathcal{H}_{E_X}, H_{E_X}, \rho_{E_X}, U)$ to it.

Similarly as the definition 1, the definition 4 is too general for practical purpose. Thus, we introduce two classes of the FQ-work extraction. The element of the first class reduces to the CP-strong work extraction, and the element of the second class reduces to the CP-unital work extraction. The first class is used in Refs. [31, 33–37];

Definition 5 (FQ-strong work extraction)**.** *Let us consider an external system $\mathcal{H}_{E_X}$ with the Hamiltonian H_{E_X}. If the set $(\mathcal{H}_{E_X}, H_{E_X}, \rho_{E_X}, U)$ satisfies the following condition, we refer to the set $(\mathcal{H}_{E_X}, H_{E_X}, \rho_{E_X}, U)$ as the FQ-strong work extraction:*

Condition FQS1 *The initial state ρ_{E_X} is a pure energy eigenstate of H_{E_X} or a mixture of pure energy eigenstates whose eigenvalues are the same.*

Condition FQS2 *The unitary U satisfies*

$$[U, H_I + H_{E_X}] = 0. \tag{3.57}$$

Lemma 4. *An arbitrary FQ-strong work extraction reduces to a CP-strong work extraction by the FQ-CP map.*

Proof: Let us take an arbitrary FQ-strong work extraction $(\mathcal{H}_{E_X}, H_{E_X}, \rho_{E_X}, U)$. By the FQ-CP map, we reduces $(\mathcal{H}_{E_X}, H_{E_X}, \rho_{E_X}, U)$ into the CP-work extraction $\{\mathcal{E}_j, w_j\}_{(\mathcal{H}_{E_X}, H_{E_X}, \rho_{E_X}, U)}$. We also take an arbitrary normalized eigenvector $|x\rangle$ of H_I with an eigenvalue h_x, and denote the spectral decomposition of H_I as $H_I = \sum_h hP_h$, where P_h is the projection to the energy eigenspace of H_I whose eigenvalue is h. Because of Condition FQS1, and because the unitary U satisfies the energy conservation (3.57), the state $\mathcal{E}_j(|x\rangle\langle x|)/p_j$ is a pure energy eigenstate of H_I or a mixture of pure energy eigenstates whose eigenvalues are the same. Note that w_j is defined as $h_{E|j} - \mathrm{Tr}[H_{E_X \rho_{E_X}}]$, by the FQ-CP map. Thus, because of Condition FQS1 and because the unitary U satisfies the energy conservation (3.57), the state $\mathcal{E}_j(|x\rangle\langle x|)/p_j$ has the energy eigenvalue $h_x - w_j$. Thus, the unnormalized state $\mathcal{E}_j(|x\rangle\langle x|)$ and the measured value w_j satisfy (3.37). Hence, the CP-work extraction $\{\mathcal{E}_j, w_j\}_{(\mathcal{H}_{E_X}, H_{E_X}, \rho_{E_X}, U)}$ is the CP-strong work extraction. □

Next, we introduce the second class of the FQ-work extraction, whose element reduces to the CP-unital work extraction by the FQ-CP map. It is given by generalizing the work storage introduced in Ref. [12].

Definition 6 (FQ-memoryless work extraction)**.** *We refer to an FQ-work extraction* $(\mathcal{H}_{E_X}, H_{E_X}, \rho_{E_X}, U)$ *which satisfies the following conditions as the FQ-memoryless work extraction:*

Condition FQM1 *The external system* E_X *is a non-degenerate system, or a composit system of a non-degenerate system* E_{X1} *and a fully degenerate system* E_{X2}*. The initial state of* E_X *is the product state of a pure energy eigenstate* $|l\rangle_{E_X1}$ *of* E_{X1} *and a mixed state* $\rho_{E_{X2}} := \sum_i p_i |i\rangle_{E_{X2}}\langle i|_{E_{X2}}$ *of* E_{X2}*, where* $\{|i\rangle_{E_{X2}}\}$ *is an orthonormal basis of* $\mathcal{H}_{E_{X2}}$*.*

Condition FQM2 *The unitary* U *is written as*

$$U = \sum_i U_{i,IE_{X1}} \otimes |i\rangle_{E_{X2}}\langle i|_{E_{X2}}, \tag{3.58}$$

where each $U_{i,IE_{X1}}$ *is the unitary on* IE_{X2} *such that the following CP-map only depends on* i *and* $l-l'$*;*

$$\mathcal{E}^i_{l,l'}(\rho_I) := \mathrm{Tr}_{E_X}[|l'\rangle_{E_{X1}}\langle l'|_{E_{X1}} U_{i,IE_{X1}}(|l\rangle_{E_{X1}}\langle l|_{E_{X1}} \otimes \rho_I) U^\dagger_{i,IE_{X1}} |l'\rangle_{E_X}\langle l'|_{E_X}]. \tag{3.59}$$

Namely, $\mathcal{E}^i_{l,l'} = \mathcal{E}^i_{l+\delta l, l'+\delta l}$ *holds for an arbitrary* δl*.*

The subsystem E_{X1} means a work storage, and the subsystem E_{X2} means a noise source. We refer to an FQ-memoryless work extraction without the noise source as the FQ-memoryless work extraction without noise. When a CP-work extraction $\{\mathcal{E}_j, w_j\}$ is reduced from an FQ-memoryless work extraction, the CP-work extraction $\{\mathcal{E}_j, w_j\}$ can be written with a probability $\{p(m)\}$ and the CP-work extractions $\{\mathcal{F}^{[m]}_j, w_j\}$ which are reduced from the FQ-memoryless work extractions without noise as follows:

$$\mathcal{E}_j = \sum_m p_m \mathcal{F}^{[m]}_j. \tag{3.60}$$

There are two points in the definition 6. First, in order to satisfy Condition FQM2, the dimension of the work storage E_{X1} should be infinite.

Second, we can interpret the FQ-memoryless work extraction as the work extraction without memory effect. Let us consider the situation that we perform CP-work extractions n times. Let the kth CP-work extraction is reduced from the FQ work extraction $(\mathcal{H}_{E_X}, H_{E_X}, \rho^{(k)}_E, U)$, and let $\rho^{(k)}_E$ be the final state of the external system of the $k-1$th work extraction. Therefore, if the FQ work extraction $(\mathcal{H}_{E_X}, H_{E_X}, \rho^{(k)}_E, U)$ is not FQ-memoryless, the kth CP-work extraction depends on the outcomes of the previous CP-work extractions. Namely, there exists a memory effect. If the FQ work extraction $(\mathcal{H}_{E_X}, H_{E_X}, \rho^{(k)}_E, U)$ is FQ-memoryless, then the memory effect does not exist, because of Condition FQM2. Thus, when we perform a CP-work extraction which is reduced from an FQ-memoryless work extraction, we don't have to initialize the external system after the projective measurement on the external system.

Lemma 5. *An arbitrary FQ-memoryless work extraction reduces to a CP-unital work extraction by the FQ-CP map.*

Proof: Because of (3.60), we only have to prove an arbitrary FQ-memoryless work extraction without noise reduces to a CP-unital work extraction. Namely, we only have to prove

$$\sum_{l'} \mathcal{E}_{l,l'}(\hat{1}_I) = \hat{1}, \text{ for any } l \tag{3.61}$$

where

$$\mathcal{E}_{l,l'}(\rho_I) := \mathrm{Tr}_{E_X}[|l'\rangle_{E_X}\langle l'|_{E_X} U(|l\rangle_{E_X}\langle l|_{E_X} \otimes \rho_I)U^\dagger |l'\rangle_{E_X}\langle l'|_{E_X}]. \tag{3.62}$$

Because of $\mathcal{E}_{l,l'} = \mathcal{E}_{l+\delta l, l'+\delta l}$ for an arbitrary δl, we obtain (3.61) as follows;

$$\sum_{l'} \mathcal{E}_{l,l'}(\hat{1}_I) = \sum_{l'} \mathcal{E}_{l',-l}(\hat{1}_I) \tag{3.63}$$

$$= \sum_{l'} \mathrm{Tr}_{E_X}[|-l\rangle_{E_X}\langle -l|_{E_X} U(|l'\rangle_{E_X}\langle l'|_{E_X} \otimes \hat{1}_I)U^\dagger |-l\rangle_{E_X}\langle -l|_{E_X}] \tag{3.64}$$

$$= \mathrm{Tr}_{E_X}[|-l\rangle_{E_X}\langle -l|_{E_X} U(\hat{1}_{E_X} \otimes \hat{1}_I)U^\dagger |-l\rangle_{E_X}\langle -l|_{E_X}] \tag{3.65}$$

$$= \hat{1}_I. \tag{3.66}$$

□

So far, we have considered the mapping from the FQ-work extraction to the CP-work extraction. How about the converse mapping? As we show in the following theorem, we can always find an FQ-work extraction which reduces to an arbitrary CP-work extraction;

Theorem 2. *For an arbitrary CP-work extraction $\{\mathcal{E}_j, w_j\}$, there exists an FQ-weak work extraction $(\mathcal{H}_{E_X}, H_{E_X}, \rho_{E_X}, U)$ which reduces to $\{\mathcal{E}_j, w_j\}$ by the FQ-CP map.*

Proof: We only have to prove that we can take an FQ work extraction $(\mathcal{H}_{E_X}, H_{E_X}, \rho_{E_X}, U)$ which can produce an arbitrary CP-work extraction $\{\mathcal{E}_j, w_j\}$. Let $\{E_{j,m}\}$ be a set of operation elements for $\{\mathcal{E}_j\}$; namely,

$$\mathcal{E}_j(\rho) = \sum_m E_{j,m}\rho E_{j,m}^\dagger \tag{3.67}$$

holds for an arbitrary state ρ. Introduce the external system E_X with an orthonormal basis set $\{|j,m\rangle_{E_X}\}$ and introduce the Hamiltonian of E_X as $H_{E_X} := \sum_j w_j P_j$, where $P_j := \sum_m |j,m\rangle_{E_X}\langle j,m|_{E_X}$. Let us define the unitary U on IE_X as

$$U|x\rangle_I|0,0\rangle_{E_X} = \sum_{j,m} E_{j,m}|x\rangle_I|j,m\rangle_{E_X}, \tag{3.68}$$

where $|0,0\rangle_{E_X}$ is an eigenstate of H_{E_X} whose eigenvalue we set to zero. Then,

$$\mathcal{E}_j(\rho) = \mathrm{Tr}_{E_X}[P_j U(\rho \otimes |0,0\rangle\langle 0,0|)U^\dagger P_j] \tag{3.69}$$

holds for arbitrary ρ. Let us prove that the set $(\mathcal{H}_{E_X}, H_{E_X}, |0,0\rangle\langle 0,0|, U)$ satisfies (3.56). Because of $H_{E_X} := \sum_j w_j P_j$ and (3.69),

$$\sum_j w_j \mathrm{Tr}\mathcal{E}_j(\rho) + \mathrm{Tr}H_I\mathcal{E}_j(\rho) = \mathrm{Tr}[(H_I + H_{E_X})U(\rho \otimes |0,0\rangle\langle 0,0|)U^\dagger] \tag{3.70}$$

holds. Thus, because of (3.35) and $\mathrm{Tr}[H_{E_X}|0,0\rangle\langle 0,0|] = 0$,

$$\mathrm{Tr}[H_I\rho] + \mathrm{Tr}[H_{E_X}|0,0\rangle\langle 0,0|] = \mathrm{Tr}[(H_I + H_{E_X})U(\rho \otimes |0,0\rangle\langle 0,0|)U^\dagger] \tag{3.71}$$

holds, and hence the set $(\mathcal{H}_{E_X}, H_{E_X}, |0,0\rangle\langle 0,0|, U)$ is an FQ work extraction which yields the CP-work extraction $\{\mathcal{E}_j, w_j\}$. □

Now, let us revisit Question 2 in the section 3.1. Because the CP-work extraction only describes the time evolution of the internal system I, we need to show the existence of the time evolution of total system IE_X such that we can know the amount of the energy gain of E_X from observing E_X. Theorem 2 guarantees the existence of the time evolution. We can realize an arbitrary CP-work extraction as the internal part of the time evolution of total system IE_X such that we can know the amount of the energy gain of E_X from observing E_X.

In the present subsection, we have formulated the FQ-work extraction, and given two classes of it. The first class is the FQ-strong work extraction, whose element reduces to the CP-strong work extraction. The second class class is the FQ-strong work extraction, whose element reduces to the CP-strong work extraction by the FQ-CP map. For the convenience of description, we refer to an FQ-work extraction which is FQ-strong and FQ-memoryless at the same time as the FQSM-work extraction. Clearly, an arbitrary FQSM-work extraction reduces to a CPSU-work extraction by the FQ-CP map. We also have shown that we can always find an FQ-work extraction which reduces to an arbitrary CP-work extraction.

For a CP-work extraction, there are many FQ-work extractions which reduces to the CP-work extraction by FQ-CP map. Thus, for practical use, it is to be desired that we can find the FQ-work extraction which has a good feature, e.g., the FQ-memoryless work extraction. In the next section, we will consider this problem for the CPSU-work extraction. To be concrete, we will give a converse mapping from the CPSU-work extraction to the FQSM-work extraction. As a by-product, we will give a powerful tool to analyze the thermodynamic features of heat engines which are described as the FQSM-work extraction or the CPSU-work extraction.

3.3 Converse mapping from the CPSU-work extraction to the FQSM-work extraction

3.3.1 Fully classical model

First of all, we introduce a model of fully classical work extraction and give the map from the semi-classical work extractions, the CPSU-work extractions or the FQSM-work extraction to the classical model.

Definition 7 (Classical work extraction)**.** *We consider a classical system $\mathcal{X}$ and its Hamiltonian which is given as a real-valued function h_X on $\mathcal{X}$. We also consider a probabilistic dynamics $T(x'|x)$ on $\mathcal{X}$, which is a transition probability, i.e., $\sum_{x'} T(x'|x) = 1$. With the probabilistic dynamics $T(x'|x)$, the initial distribution $P(x)$ becomes the final distribution as in $P'(x') := \sum_x T(x'|x)P(x)$. Because of the energy conservation the amount of the extracted work between the initial and final states x and x' is $w_{x,x'} = h_X(x) - h_X(x')$. An arbitrary value w of extracted work is realized with the probability $\sum_{x,x'} P(x)T(x'|x)\delta_{h_X(x)-h_X(x'),w}$. When the transition probability is a bi-stochastic matrix, i.e., $\sum_x T(x'|x) = 1$ holds, we refer to $T(x'|x)$ as a classical unital work extraction.*

This model includes the previous fully classical scenario, in which we extract work from classical systems. For example, the set up of the Jarzynski equality [7] is a special case that $T(x'|x)$ is deterministic and unital. The classical unital work extractions correspond to the classical work extractions without feedback, and the classical non-unital work extractions correspond to the classical work extractions with feedback. We can map an arbitrary CP-work extraction to a classical model as follows:

Definition 8 (classical description)**.** *Let us perform a CP-work extraction $\{\mathcal{E}_j, w_j\}$ on an arbitrary classical state, which is written as $\rho_I = \sum_x P(x)|x\rangle\langle x|$, where $\{|x\rangle\}_{x\in\mathcal{X}}$ is the energy eigenbasis of H_I. Let us take a* *classical system whose set of states is $\mathcal{X}$ and whose hamiltonian $h(x)$ as $h(x) := \langle x|H_I|x\rangle$. We refer to the following bi-stochastic matrix $T_{\{\mathcal{E}_j,w_j\}}(x'|x)$ as the classical description of the CP-work extraction $\{\mathcal{E}_j, w_j\}$:*

$$T_{\{\mathcal{E}_j,w_j\}}(x'|x) := \sum_j \langle x'|\mathcal{E}_j(|x\rangle\langle x|)|x'\rangle \tag{3.72}$$

We refer to the map from the CP-work extraction to its classical description as CP-C map. By using the FQ-CP map and the CP-C map at the same time, we can define the classical description $T_{(\mathcal{H}_{E_X},H_{E_X},\rho_{E_X},U)}(x'|x)$ of an FQ-work extraction;

$$T_{(\mathcal{H}_{E_X},H_{E_X},\rho_{E_X},U)}(x'|x) := T_{\{\mathcal{E}_j,w_j\}_{(\mathcal{H}_{E_X},H_{E_X},\rho_{E_X},U)}}(x'|x). \tag{3.73}$$

The relationship between a CP-work extraction and its classical description is shown as in the following lemma:

Lemma 6. *Let us perform an arbitrary CP-work extraction $\{\mathcal{E}_j, w_j\}$ on an arbitrary classical state $\rho_I = \sum_x P(x)|x\rangle\langle x|$, where $\{|x\rangle\}_{x\in\mathcal{X}}$ is the energy eigenbasis of H_I. The CP-work extraction and its classical description have the same average of the extracted work;*

$$\sum_j w_j \mathrm{Tr}[\mathcal{E}_j(\rho_I)] = \sum_{x,x'} P(x)T_{\{\mathcal{E}_j,w_j\}}(x'|x)w_{x,x'}. \tag{3.74}$$

When the CP-work extraction is CP-strong, the CP-strong work extraction and its classical description have the same distribution of the extracted work;

$$\sum_j \mathrm{Tr}[\mathcal{E}_j(\rho_I)]\delta_{w,w_j} = \sum_{x,x'} P(x)T_{\{\mathcal{E}_j,w_j\}}(x'|x)\delta_{h(x)-h(x'),w}. \tag{3.75}$$

When the CP-work extraction is CP-unital, its classical description is also unital, i.e., $\sum_x T_{\{\mathcal{E}_j,w_j\}}(x'|x) = 1$ holds. Similarly, an arbitrary FQ-strong work extraction and its classical description have the same distribution of the extracted work;

$$\sum_j \mathrm{Tr}[\mathcal{E}_j(\rho_I)]\delta_{w_j,w} = \sum_{x,x'} P(x)T_{(\mathcal{H}_{E_X},H_{E_X},\rho_{E_X},U)}(x'|x)\delta_{h(x)-h(x'),w}, \tag{3.76}$$

and an arbitrary FQ-memoryless work extraction's classical description is unital.

Proof of Lemma 6: Because of (3.35) and $\rho_I = \sum_x P(x)|x\rangle\langle x|$, we obtain (3.74) as follows;

$$\begin{aligned}
\sum_j w_j \mathrm{Tr}[\mathcal{E}_j(\rho_I)] &\overset{(a)}{=} \mathrm{Tr}[H_I\rho_I] - \sum_j \mathrm{Tr}[H_I\mathcal{E}_j(\rho_I)], &(3.77)\\
&= \sum_{x'}\langle x'|H_I\rho_I|x'\rangle - \sum_{x'}\sum_j \langle x'|H_I\mathcal{E}_j(\rho_I)|x'\rangle &(3.78)\\
&\overset{(b)}{=} \sum_{x,x'} P(x)\langle x'|H_I|x\rangle\langle x|x'\rangle - \sum_{x,x'}\sum_j P(x)\langle x'|H_I\mathcal{E}_j(|x\rangle\langle x|)|x'\rangle, &(3.79)\\
&\overset{(c)}{=} \sum_x P(x)h(x) - \sum_{x,x'} P(x)h(x')T_{\{\mathcal{E}_j,w_j\}}(x'|x), &(3.80)\\
&\overset{(d)}{=} \sum_{x,x'} P(x)T_{\{\mathcal{E}_j,w_j\}}(x'|x)w_{x,x'} &(3.81)
\end{aligned}$$

where the equality (a) follows from (3.35), the equality (b) follows from $\rho_I = \sum_x P(x)|x\rangle\langle x|$, the equality (c) follows from $H_I = \sum_x h(x)|x\rangle\langle x|$ and (3.72), the equality (d) follows from the definition of $w_{x,x'}$.

Similarly, we obtain (3.75) as follows;

$$\sum_j \mathrm{Tr}[\mathcal{E}_j(\rho_I)]\delta_{w,w_j} = \sum_j \sum_{x'} \langle x'|\mathcal{E}_j(\rho_I)|x'\rangle \delta_{w,w_j} \tag{3.82}$$

$$\overset{(a)}{=} \sum_j \sum_{x,x'} P(x)\langle x'|\mathcal{E}_j(|x\rangle\langle x|)|x'\rangle \delta_{w,w_j} \tag{3.83}$$

$$\overset{(b)}{=} \sum_j \sum_{x,x'} P(x)\langle x'|\mathcal{E}_j(|x\rangle\langle x|)|x'\rangle \delta_{w_j,h(x)-h(x')}\delta_{w,w_j} \tag{3.84}$$

$$= \sum_j \sum_{x,x'} P(x)\langle x'|\mathcal{E}_j(|x\rangle\langle x|)|x'\rangle \delta_{w_j,h(x)-h(x')}\delta_{w,h(x)-h(x')} \tag{3.85}$$

$$\overset{(c)}{=} \sum_j \sum_{x,x'} P(x)\langle x'|\mathcal{E}_j(|x\rangle\langle x|)|x'\rangle \delta_{w,h(x)-h(x')} \tag{3.86}$$

$$\overset{(d)}{=} \sum_{x,x'} P(x) T_{\{\mathcal{E}_j,w_j\}}(x'|x)\delta_{h(x)-h(x'),w}. \tag{3.87}$$

where the equality (a) follows from $\rho_I = \sum_x P(x)|x\rangle\langle x|$, the equalities (b) and (c) follow from (3.37), and the equality (d) follows from (3.72). Because an arbitrary FQ-strong work extraction reduces to a CP-strong work extraction by the FQ-CP map, the equation (3.76) also holds.

Finally, we obtain $\sum_x T_{\{\mathcal{E}_j,w_j\}}(x'|x) = 1$ for an arbitrary CP-unital work extraction $\{\mathcal{E}_j, w_j\}$, as follows;

$$\sum_x T_{\mathcal{E}_j,w_j}(x'|x) = \sum_x \sum_j \langle x'|\mathcal{E}_j(|x\rangle\langle x|)|x'\rangle \tag{3.88}$$

$$= \langle x'|\sum_j \mathcal{E}_j(\sum_x |x\rangle\langle x|)|x'\rangle \tag{3.89}$$

$$= \langle x'|\sum_j \mathcal{E}_j(\hat{1}_I)|x'\rangle \tag{3.90}$$

$$= \langle x'|\hat{1}_I|x'\rangle = 1, \tag{3.91}$$

where $\hat{1}_I$ is the identity operator of I. Because an arbitrary FQ-memoryless work extraction reduces to a CP-unital work extraction by FQ-CP map, and thus the classical description of an arbitrary FQ-memoryless work extraction is also unital. □

3.3.2 Converse mapping from the CPSU-work extraction to the FQSM-work extraction

As we show in the following theorem, for an arbitrary CPSU-work extraction, we can always find an FQSM-work extraction whose classical description is the same as the classical description of the CPSU-work extraction.

Theorem 3. *For an arbitrary CPSU-work extraction $\{\mathcal{E}_j, w_j\}$, there exists an FQSM-work extraction $(\mathcal{H}_{E_X}, H_{E_X}, \rho_{E_X}, U)$ which satisfies*

$$T_{(\mathcal{H}_{E_X},H_{E_X},\rho_{E_X},U)}(x'|x) = T_{\{\mathcal{E}_j,w_j\}}(x'|x). \tag{3.92}$$

Lemma 6 guarantees that two CP-strong work extractions whose classical descriptions are the same have the same distribution of the extracted work. Thus, Theorem 3 guarantees that for an arbitrary CPSU-work

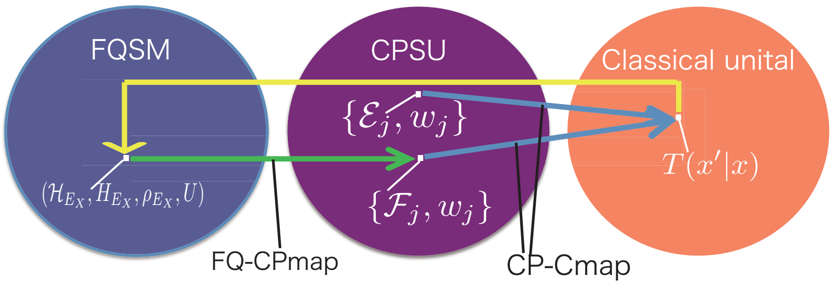

Figure 3.1: Schematic diagram of converse mapping from CPSU to FQSM. Theorem 3 guarantees that for an arbitrary CPSU-work extraction $\{\mathcal{E}_j, w_j\}$, we can always find an FQSM-work extraction $(\mathcal{H}_{E_X}, H_{E_X}, \rho_{E_X}, U)$ which is reduced to CPSU-work extraction $\{\mathcal{F}_j, w_j\}$ whose distribution of the extracted work is the same as $\{\mathcal{E}_j, w_j\}$. Lemma 7 and Corollary 2 guarantee that for an arbitrary classical work extraction $T(x'|x)$ we can always find an FQSM-work extraction $(\mathcal{H}_{E_X}, H_{E_X}, \rho_{E_X}, U)$ and a CPSU-work extraction $\{\mathcal{F}_j, w_j\}$ whose classical description is $T(x'|x)$.

extraction $\{\mathcal{E}_j, w_j\}$, we can always find an FQSM-work extraction $(\mathcal{H}_{E_X}, H_{E_X}, \rho_{E_X}, U)$ which is reduced to CPSU-work extraction $\{\mathcal{F}_j, w_j\}$ whose distribution of the extracted work is the same as $\{\mathcal{E}_j, w_j\}$ (Fig.3.3.2).

Theorem 3 can be easily shown by using the following lemma;

Lemma 7. *There exists an FQSM-work extraction which has the same classical description as an arbitrary classical model. Namely, for an arbitrary bi-stochastic matrix $T(x'|x)$, there exists an FQSM-work extraction $(\mathcal{H}_{E_X}, H_{E_X}, \rho_{E_X}, U)$ which satisfies $T(x'|x) = T_{(\mathcal{H}_{E_X}, H_{E_X}, \rho_{E_X}, U)}(x'|x)$.*

Lemma 7 has an important corollary;

Corollary 2. *We can always find a CPSU-work extraction $\{\mathcal{F}_j, w_j\}$ whose classical description is the same as an arbitrary classical work extraction $T(x'|x)$.*

We can give the CPSU-work extraction as $\{\mathcal{F}_j, w_j\} := \{\mathcal{E}_j, w_j\}_{(\mathcal{H}_{E_X}, H_{E_X}, \rho_{E_X}, U)}$. Note that a CPSU-work extraction and its classical description have the same distribution of the extracted work. Thus, for an arbitrary classical work extraction, we can take a CPSU-work extraction whose probabilistic distribution of the extracted work is the same as that of the classical work extraction. This fact is very useful; we can analyze classical models as a substitution for quantum heat engines, which are described as the CPSU-work extraction. We use the fact in Chapter 4.

We prove Theorem 3 and Lemma 7 in the next subsection. As a by-product, we will clarify the relationship between our work extraction scenario and the semi-classical work extraction scenario.

3.3.3 Relationship between our scenario and semi-classical scenario

In the same way as the definition 8, we can give the classical description of the semi-classical work extraction.

Definition 9 (classical description of semi-classical work extraction)**.** *Let us perform a semi-classical work extraction U_I on an arbitrary classical state, which is written as $\rho_I = \sum_x P(x)|x\rangle\langle x|$, where $\{|x\rangle\}_{x\in\mathcal{X}}$ is the energy eigenbasis of H_I. Let us take a classical system whose set of states is $\mathcal{X}$ and whose hamiltonian $h(x)$ as $h(x) := \langle x|H_I|x\rangle$. We refer to the following bi-stochastic matrix $T_{U_I}(x'|x)$ as the classical description of the semi-classical work extraction U_I:*

$$T_{U_I}(x'|x) := \langle x'|U_I|x\rangle\langle x|U_I^\dagger|x'\rangle \tag{3.93}$$

We refer to the map from the semi-classical extraction to its classical description as U-C map.

The relationship between our scenario and semi-classical scenario is given by the following lemma. It is also used to prove Theorem 3 and Lemma 7.

Lemma 8. *There exists an FQSM-work extraction without noise* $(\mathcal{H}_{E_X}, H_{E_X}, \rho_{E_X}, U)$ *which has the same classical description as an arbitrary semi-classical work extraction with the time evolution* U_I*. Namely,* $T_{U_I}(x'|x) = T_{(\mathcal{H}_{E_X}, H_{E_X}, \rho_{E_X}, U)}(x'|x)$ *holds. Conversely, for an arbitrary FQSM-work extraction without noise* $(\mathcal{H}_{E_X}, H_{E_X}, \rho_{E_X}, U)$*, there exists a semi-classical work extraction* U_I *which satisfies* $T_{U_I}(x'|x) = T_{(\mathcal{H}_{E_X}, H_{E_X}, \rho_{E_X}, U)}(x'|x)$*.*

The relationship among our scenario, the semi-classical work extraction, and the classical unital work extraction can be drawn as Fig.3.2. There exists one-to-one correspondence between the FQSM work extractions without noise and the semi-classical work extractions, in the sense those classical descriptions are the same. There also exists one-to-one correspondence between the FQSM work extractions and the classical unital work extractions. In the above sense, the semi-classical work extraction and the classical unital work extraction are included in our work extraction scenario.

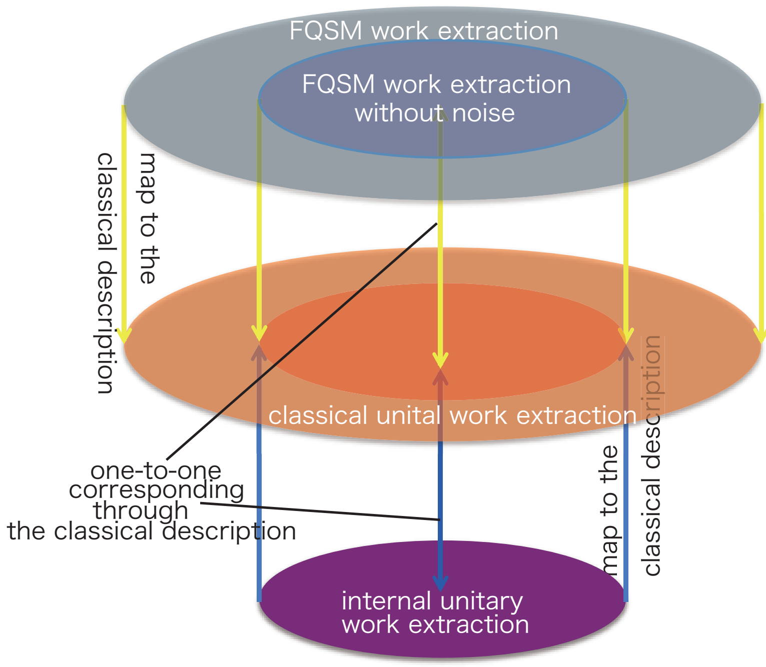

Figure 3.2: The schematic graph of the relationships among the FQSM work extraction, the internal work extraction and the fully classical work extraction. There exists one-to-one correspondence between the FQSM work extractions without noise and the semi-classical work extractions, in the sense those classical descriptions are the same. There also exists one-to-one correspondence between the FQSM work extraction and the classical unital work extraction

Let us prove Theorem 3, Lemma 7 and Lemma 8. We firstly prove Lemma 8, and secondly prove Lemma 7, and finally prove Theorem 3.

Proof of Lemma 8: We first prove the first statement; we fix an arbitrary unitary transformation U_I. Let us give the FQSM-work extraction without noise $(\mathcal{H}_{E_X}, H_{E_X}, \rho_{E_X}, V)$ which satisfies $T_{U_I}(x'|x) = T_{(\mathcal{H}_{E_X}, H_{E_X}, \rho_{E_X}, V)}(x'|x)$. We choose a suspended weight as the external system. Namely, the Hilbert space $\mathcal{H}_{E_X}$ is $L_2(R)$ and its Hamiltonian H_{E_X} is $\sum_{j\in\mathcal{R}} j|j\rangle\langle j|$, where $\{|j\rangle\}_{j\in\mathcal{R}}$ is an orthonomal basis set of $\mathcal{H}_{E_X}$.

Then, the following $(\mathcal{H}_{E_X}, H_{E_X}, \rho_{E_X}, V)$ is the memoryless work extraction without noise which we are seeking;

$$
\begin{aligned}
V|j\rangle|x\rangle &:= \sum_y u_{y,x}|j+h(x)-h(y)\rangle|y\rangle, \text{ where } u_{y,x} := \langle y|U_I|x\rangle, && (3.94)\\
w_j &:= j. && (3.95)
\end{aligned}
$$

Because the unitary V clearly commutes with $H_I + H_{E_X}$ and because the initial state $|0\rangle$ of the external system is a pure eigenstate, $(\mathcal{H}_{E_X}, H_{E_X}, \rho_{E_X}, V)$ is an FQ-strong work extraction. Because of (3.94), the CP-map

$$
\mathcal{E}_j^{j_0}(\rho) := \mathrm{Tr}_{E_X}[|j\rangle\langle j|V(|j_0\rangle\langle j_0| \otimes \rho)V^\dagger|j\rangle\langle j|] \qquad (3.96)
$$

depends only on $j - j_0$, and thus $(\mathcal{H}_{E_X}, H_{E_X}, \rho_{E_X}, V)$ is an FQ-memoryless work extraction without noise. Thus, $(\mathcal{H}_{E_X}, H_{E_X}, \rho_{E_X}, V)$ is an FQSM-work extraction. Finally, we show $T_{U_I}(x'|x) = T_{(\mathcal{H}_{E_X}, H_{E_X}, \rho_{E_X}, V)}(x'|x)$;

$$
\begin{aligned}
T_{(\mathcal{H}_{E_X}, H_{E_X}, \rho_{E_X}, V)}(x'|x) &= \sum_j \mathrm{Tr}[\langle x'|\mathcal{E}_j(|x\rangle\langle x|)|x'\rangle] && (3.97)\\
&= \sum_j \langle x'|\mathrm{Tr}_{E_X}[|j\rangle\langle j|V(|0\rangle\langle 0| \otimes |x\rangle\langle x|)V^\dagger|j\rangle\langle j|]|x'\rangle && (3.98)\\
&= \mathrm{Tr}_{E_X}[\langle x'|V(|0\rangle\langle 0| \otimes |x\rangle\langle x|)V^\dagger|x'\rangle] && (3.99)\\
&= |u_{x',x}|^2 = \langle x'|U_I|x\rangle\langle x|U_I^\dagger|x'\rangle = T_{U_I}(x'|x). && (3.100)
\end{aligned}
$$

Next, we prove the second statement. We take an arbitrary FQSM-work extraction without noise $(\mathcal{H}_{E_X}, H_{E_X}, \rho_{E_X}, U)$. Note that an arbitrary FQSM-work extraction $(\mathcal{H}_{E_X}, H_{E_X}, \rho_{E_X}, U)$ can be written as follows:

$$
U|l\rangle_{E_X}|x\rangle_I = \sum_y f_{x,y}|l + \Delta(h(x)-h(y))\rangle_{E_X}|y\rangle_I, \qquad (3.101)
$$

where $f_{x,y}$ is a matrix of the complex numbers, and $|l + \Delta(x,y)\rangle$ is the energy eigen vector of H_{E_X} with its energy eigenvalue $e_l + h(x) - h(y)$, and where e_l is the energy eigenstate of $|l\rangle_{E_X}$. Then, $V_I|x\rangle := \sum_y f_{x,y}|y\rangle$ is the unitary transformation on $\mathcal{H}_I$ which we are seeking. Because $T_{V_I}(x'|x) = T_{(\mathcal{H}_{E_X}, H_{E_X}, \rho_{E_X}, U)}(x'|x) = f(x,x')$ clearly holds, we only have to prove that V_I is unitary. In order to show the unitarity of V_I, it is enough to show the unitarity of $f_{x,y}$. Because U is unitary, $UU^\dagger = \hat{1}$ and $U^\dagger U = \hat{1}$ hold. The equation $UU^\dagger = \hat{1}$ yields the equation $\sum_y f_{x,y} f^*_{x',y} = \delta_{x,x'}$, as follows;

$$
\begin{aligned}
UU^\dagger &= \sum_{x,y,l,x',y',l'} f_{x,y} f^*_{x',y'}|l + \Delta(h(x)-h(y))\rangle|y\rangle\langle l' + \Delta(h(x)-h(y))|\langle y'|\delta_{x,x'}\delta_{l,l'} && (3.102)\\
\langle L|\langle y|UU^\dagger|L'\rangle|y'\rangle &= \sum_{x,l} f_{x,y} f^*_{x,y'}\delta_{L,l+\Delta(h(x)-h(y))}\delta_{L',l+\Delta(h(x)-h(y'))} && (3.103)\\
&= \sum_x f_{x,y'} f^*_{x,y'}\delta_{L',L+\Delta(h(y)-h(y'))} && (3.104)
\end{aligned}
$$

Thus, in order to $\langle L|\langle y|UU^\dagger|L'\rangle|y'\rangle = \delta_{y,y'}\delta_{L,L'}$, the equation $\sum_x f_{x,y} f^*_{x,y'} = \delta_{y,y'}$ has to hold. Similary, the equation $U^\dagger U = \hat{1}$ yields the equation $\sum_y f^*_{x',y} f_{x,y} = \delta_{x,x'}$. Thus, the matrix $f_{x,y}$ is unitary, and thus V_I is also unitary. □

Proof of Lemma 7: We can express the bi-stochastic matrix $T(x'|x)$ with the probability $\{p(i)\}$ and permutation matrices $D^{[i]}_{x',x}$ as $T(x'|x) = \sum_i p(i) D^{[i]}_{x',x}$ [60]. Because the permutation matrix is unitary, there exists an

FQSM-work extraction without noise $(\mathcal{H}_{E_{X1}}, H_{E_{X1}}, \rho_{E_{X1}}, U^{[i]}_{IE_{X1}})$ which satisfies $D^{[i]}_{x',x} = T_{(\mathcal{H}_{E_{X1}}, H_{E_{X1}}, \rho_{E_{X1}}, U^{[i]}_{IE_{X1}})}(x'|x)$. Let us substitute $U^{[i]}_{IE_{X1}}$ for $U_{i,IE_{X1}}$ of (3.58). Then, the FQSM-work extraction $(\mathcal{H}_{E_X}, H_{E_X}, \rho_{E_X}, U)$ in the definition 6 becomes the FQSM-work extraction whose classical description satisfies $T(x'|x) = T_{(\mathcal{H}_{E_X}, H_{E_X}, \rho_{E_X}, U)}(x'|x)$. □

Proof of Theorem 3: The classical description $T_{\{\mathcal{E}_j, w_j\}}(x'|x)$ is a bi-stochastic matrix, we can take the FQSM-work extraction $(\mathcal{H}_{E_X}, H_{E_X}, \rho_{E_X}, U)$ which satisfies (3.92), because of Lemma 7. □

In the present chapter, we have reconsidered the formulation of the work extraction from the viewpoint of quantum measurement theory, and clarified a serious conflict between the semi-classical scenario and the fully quantum scenario. We gives a trade-off inequality which means that we have to destroy the coherence of the thermodynamic system in order to know the amount of the extracted energy; namely, a work extraction must be a measurement. Based on the fact, we have formulated the work extractions as a measurement process, and putted the previous formulations in order in a hierarchical structure. As a by-product, our formulation gives us a powerful tool to analyze the thermodynamic features of quantum heat engines; when the initial state is classical, we can analyze the classical model as a substitution for quantum heat engines.

Chapter 4

Finite-size Thermodynamics

In the present chapter, we give a useful method clarifying thermodynamic features of the mesoscopic system, which consists of a very large, but finite number of particles. To deal with finitely large values of particle number n, we need two analytical tools in the information theory; namely, the information geometry [59] and the strong large deviation theory [46, 47]. Using these tools, we firstly rederive a thermodynamical upper bound for the efficiency of finite-size heat engines with two heat baths that are composed of n identical particles. Next, we asymptotically expand the upper bound in terms of $q_n := Q_{H,n}/n$, where the $Q_{H,n}$ is the extracted heat from the hot heat bath. In the case that the heat baths ' particle are uncorrelated each others, we can construct a concrete CPSU-work extraction $\{\overline{\mathcal{E}}_j, w_j\}$ whose efficiency coincides with the upper bound up to the term of the first order q_n; namely, thermodynamics gives an approximation to the optimal efficiency which is accurate up to the the order of q_n in general. In the case that $Q_{H,n}$ is a non-decreasing function of n, the efficiency of $\{\overline{\mathcal{E}}_j, w_j\}$ coincides the upper bound up to the term of the second order q_n^2; in that case, thermodynamics gives an approximation to the optimal efficiency which is accurate up to the the order of q_n^2.

4.1 Carnot's Theorem for finite-size systems

4.1.1 Heat engine with n-particle heat baths

As the internal system, let us consider the following four-body system; the working body S, the hot and cold heat baths B_H and B_L respectively, and a parameter controller. We focus on the heat baths that are composed of n paticles each of which has d energy levels. We treat the particles as n qudits; we consider only the particles' internal degrees of freedom, *not* their positions and momenta. We also treat the heat engine S as a D-level system. Thus, our setup includes finite-particle heat engines; e.g., $D = d^l$ when the heat engine S is composed of l particles with d-levels.

The Hamiltonian of the internal system is written as

$$H_I = \sum_{\lambda} H_{SB_HB_L}(\lambda) \otimes |\lambda_{S_C}\rangle\langle\lambda_{S_C}|, \tag{4.1}$$

$$H_{SB_HB_L}(\lambda) = H_S(\lambda) + H_{SB_H}(\lambda) + H_{SB_L}(\lambda) + H_{B_H} + H_{B_L} \tag{4.2}$$

The system Hamiltonian $H_S(\lambda)$ describes a mechanical operation on S through the parameter λ, e.g., the volume of the gas or an applied magnetic field. Similary, $H_{SB_H}(\lambda)$ is the interaction Hamiltonian between S and B_H, while $H_{SB_L}(\lambda)$ is the one between S and B_L. They describe, for example, the attachment or detachment of B_H and B_L to S.

On the above internal system, we perform the CPSU-work extraction $\{\mathcal{E}_j, w_j\}$ on the internal system. Initially, the system S is in an arbitrary state ρ_{ini}^S, the controller S_C is in a pure state $|\lambda_{\mathrm{i}}\rangle$, and the heat baths B_H and B_L are in Gibbs states at the inverse temperatures β_H and β_L, respectively. We assume that both heat baths B_H and B_L are initially in Gibbs state $\rho_{\mathrm{G},\beta_H}(H_{B_H}) := \exp(-\beta_H H_{B_H})/\mathrm{tr}[\exp(-\beta_H H_{B_H})]$ and $\rho_{\mathrm{G},\beta_L}(H_{B_L}) := \exp(-\beta_L H_{B_L})/\mathrm{tr}[\exp(-\beta_L H_{B_L})]$.

In order to consider cyclic operations, we also assume that the states of the working body S and the controller S_C after the CPSU-work extraction $\{\mathcal{E}_j, w_j\}$ are the same as the initial states for every measurement outcome j;

$$\mathrm{tr}_{B_H B_L}[\mathcal{E}_j(\rho_{\mathrm{ini}})] = \rho_{\mathrm{ini}}^S \otimes |\lambda_{\mathrm{i}}\rangle\langle\lambda_{\mathrm{i}}| \ \text{ for any } \ j. \tag{4.3}$$

Thus, in our model, the cyclic thermodynamical process is the transformation of the internal sytem from the initial state $\rho_{\mathrm{ini}} := \rho_{\mathrm{ini}}^S \otimes \rho_{\mathrm{G},\beta_H}(H_{B_H}) \otimes \rho_{\mathrm{G},\beta_L}(H_{B_L})$ to the final state $\rho_{\mathrm{fin}}^j := \mathcal{E}_j(\rho_{\mathrm{ini}})/p_j$ with the probability $p_j := \mathrm{tr}[\mathcal{E}_j(\rho_{\mathrm{ini}})]$. We refer to the cyclic thermodynamic process with the n-particle heat baths as an n-particle thermodynamic operation. The average work $W_{\mathrm{ext}}^{(n)}(\{\mathcal{E}_j, w_j\})$ extracted during the n-particle thermodynamic operation $\{\mathcal{E}_j, w_j\}$ is given by the average of w_j, which is equal to the energy loss of the internal system:

$$W_{\mathrm{ext}}^{(n)}(\{\mathcal{E}_j, w_j\}) := \sum_j p_j w_j = \mathrm{tr}[H_I(\rho_{\mathrm{ini}} - \sum_j p_j \rho_{\mathrm{fin}}^j)]. \tag{4.4}$$

The heat $Q_{H,n}(\{\mathcal{E}_j, w_j\})$ extracted from B_H to S is given by the average energy loss of B_H:

$$Q_{H,n}(\{\mathcal{E}_j, w_j\}) := \mathrm{tr}[H_{B_H}(\rho_{\mathrm{ini}}^{B_H} - \sum_j p_j \rho_{\mathrm{fin}}^{j,B_H})], \tag{4.5}$$

where $\rho_{\mathrm{fin}}^{j,B_H} = \mathrm{tr}_{SB_L S_C}[\rho_{\mathrm{fin}}^j]$. The efficiency $\eta^{(n)}(\{\mathcal{E}_j, w_j\})$ is defined as

$$\eta^{(n)}(\{\mathcal{E}_j, w_j\}) := \frac{W_{\mathrm{ext}}^{(n)}(\{\mathcal{E}_j, w_j\})}{Q_{H,n}(\{\mathcal{E}_j, w_j\})}. \tag{4.6}$$

4.1.2 Upper bound for the efficiency of heat engines with n-particle heat baths

In the following theorem, we give a general upper bound for the efficiency, using the relative entropy $D(\rho||\sigma) := \mathrm{tr}[\rho(\log\rho - \log\sigma)]$, the energy average $U(\beta, H) := \mathrm{tr}[\rho_{\mathrm{G},\beta}(H)H]$ and the von Neumann entropy $S(\beta, H) = S(\rho_{\mathrm{G},\beta}(H)) := -\mathrm{tr}[\rho_{\mathrm{G},\beta}(H)\log\rho_{\mathrm{G},\beta}(H)]$, of each particle of the heat baths:

Theorem 4 (General upper bound of efficiency)**.** *When an n-particle thermodynamic operation $\{\mathcal{E}_j, w_j\}$ has a constant extracted heat $Q_{H,n}$, the efficiency $\eta^{(n)}(\{\mathcal{E}_j, w_j\})$ is bounded as follows;*

$$\eta^{(n)}(\{\mathcal{E}_j, w_j\}) \le \left(1 - \frac{\beta_H}{\beta_L}\right) - \frac{D(\rho_{\mathrm{G},\beta'_H}(H_{B_H})||\rho_{\mathrm{G},\beta_H}(H_{B_H})) + D(\rho_{\mathrm{G},\beta'_L}(H_{B_L})||\rho_{\mathrm{G},\beta_L}(H_{B_L}))}{\beta_L Q_{H,n}}, \tag{4.7}$$

where the real numbers β'_H and β'_L are determined by

$$U(\beta_H, H_{B_H}) - U(\beta'_H, B_H) = Q_{H,n}, \tag{4.8}$$

$$S(\beta'_H, H_{B_H}) + S(\beta'_L, H_{B_L}) = S(\beta_H, H_{B_H}) + S(\beta_L, H_{B_L}). \tag{4.9}$$

The upper bound (4.7) is an extension of Carnot's inequality. It is not be the optimal bound, but it is a good approximation of the optimal bound in the case that the heat baths' particle are uncorrelated each others; the Hamiltonian of the n-particle heat baths are written as $H_{B_H} = \sum_{k=1}^n H_{B_H}^{[k]}$ and $H_{B_L} = \sum_{k=1}^n H_{B_L}^{[k]}$, where $H_{B_H}^{[k]} = H_{B_L}^{[k]} := H_B$ are the Hamiltonian of the kth particle of B_H and B_L, respectively. The upper bound (4.7) approximates the optimal bound up to the order of q_n^2. To see this, we next asymptotically expand (4.7). In order to describe the asymptotic expansion, we introduce the energy variance and the energy skewness of each particle of the heat baths: $\sigma^2(\beta) := \mathrm{tr}[\rho_\beta H_B^2] - \mathrm{tr}[\rho_\beta H_B]^2$ and $\gamma_1(\beta) = \mathrm{tr}[\rho_{\mathrm{G},\beta}(H_B - U(\beta))^3]/\sigma^3(\beta)$.

Theorem 5 (Extended Carnot's Theorem)**.** *When n-particle thermodynamic operations $\{\{\mathcal{E}_j, w_j\}\}_{n=1}^\infty$ have extracted heats $\{Q_{H,n}\}_{n=1}^\infty$ satisfying $\lim_{n\to\infty} Q_{H,n}/n = 0$, the upper bound (4.7) has an asymptotic expansion as follows:*

$$\eta^{(n)}(\{\mathcal{E}_j, w_j\}) \le \left(1 - \frac{\beta_H}{\beta_L}\right) - \sum_{k=1}^\infty c_{\beta_H}^{(k)} q_n^k, \tag{4.10}$$

where $q_n := Q_{H,n}/n$ and

$$c_{\beta_H,\beta_L}^{(1)} := \left(\frac{1}{2\beta_H^2\sigma^2(\beta_H)} + \frac{1}{2\beta_L^2\sigma^2(\beta_L)}\right)\frac{\beta_H^2}{\beta_L} \tag{4.11}$$

$$c_{\beta_H,\beta_L}^{(2)} := \left(-\frac{\gamma_1(\beta_H)}{6\beta_H^3\sigma^3(\beta_H)} + \frac{\gamma_1(\beta_L)}{6\beta_L^3\sigma^3(\beta_L)} + \frac{1}{2\beta_L^4\sigma^4(\beta_L)} + \frac{1}{2\beta_H^2\beta_L^2\sigma^2(\beta_H)\sigma^2(\beta_L)}\right)\frac{\beta_H^3}{\beta_L}. \tag{4.12}$$

On the other hand, for an arbitrary sequence of real numbers $\{\tilde{q}_n\}$ which satisfy $\tilde{q}_n \to 0$ at the limit $n \to \infty$, we can take the n-particle thermodynamic operations $\{\overline{\mathcal{E}}_j, w_j\}$ whose extracted heats $\{Q_{H,n}\}$ satisfy $\frac{q_n}{\tilde{q}_n} := \frac{Q_{H,n}}{n\tilde{q}_n} \to 1$ at the limit $n \to \infty$ and

$$\eta^{(n)}(\{\overline{\mathcal{E}}_j, w_j\}) = \left(1 - \frac{\beta_H}{\beta_L}\right) - c_{\beta_H,\beta_L}^{(1)} q_n - c_{\beta_H,\beta_L}^{(2)} q_n^2 - d_{\beta_H,\beta_L}^{(1)} \frac{q_n}{n} + O\left(\frac{q_n^2}{\sqrt{n}}\right) + O\left(q_n^3\right), \tag{4.13}$$

where

$$d_{\beta_H,\beta_L}^{(1)} := \left((\frac{\gamma_1(\beta_H)}{2\beta_H\sigma(\beta_H)} + \frac{1}{\beta_H^2\sigma^2(\beta_H)})^2 + (\frac{\gamma_1(\beta_L)}{2\beta_L\sigma(\beta_L)} + \frac{1}{\beta_L^2\sigma^2(\beta_L)})^2 \right)\frac{\beta_H^2}{\beta_L}. \tag{4.14}$$

The inequality (4.10) is simply the Taylor expansion of (4.7) in terms of $q_n = Q_{H,n}/n$. However, because there exists $\{\overline{\mathcal{E}}_j, w_j\}$ which satisfies (4.13), the inequality approximates the upper limit up to the order of q_n. When the $Q_{H,n}$ is a non-decreasing function of n, the inequality approximates the upper limit up to the order of q_n^2. When the $Q_{H,n}$ is a decreasing function of n, the inequality does not approximate the upper limit up to the order of q_n^2, because of the term of order q_n/n. However, $Q_{H,n}$ is naturaly non-decreasing of n, because macroscopic heat engines treat an extremely larger amount of energies than microscopic heat engines. Thus, we can expect the inequality (4.10) approximates the upper limit up to the second order, in most cases. Note that both of (4.10) and (4.13) converge into Carnot's inequality at the limit of $n \to \infty$; Thus, Theorem 5 gives a statistical mechanical proof of the achievability of the Carnot efficiency at the macroscopic limit, as a corollary.

4.1.3 Accuracy of thermodynamics in finite-size systems

As we show in Appendix C, we can derive (4.7) from thermodynamics; Theorem 4 means a microscopic derivation of thermodynamical upper bound of the efficiency of heat engines with finite-size heat baths. Thus, Theorem 5 means that the difference between the thermodynamical upper bound and the optimal efficiency is at most in the order of $O(q_n^2)$ in case of the particles in each heat baths does not interact with each others. (Note: Theorem 4 holds even for the case that the particles in each heat baths interacts with each others, unlike Theorem 5.)

In order to illustrate the above fact, let us consider a concrete model, and plot Carnot's bound, the thermodynamical upper bound (4.7) and the asymptotic expansion (4.13). (Fig. 4.1.3 and Fig.4.1.3) As the internal system, we take the heat baths which are the n-qubit systems, and the working body which is the 3-qubit system. The Hamiltonian of the combined system SB_HB_L as follows:

$$H_{SB_HB_L} = H_S + H_{B_H} + H_{B_L} \tag{4.15}$$

$$H_S = 2(\sigma_z^{[1]} + \sigma_z^{[2]} + \sigma_z^{[3]}) \tag{4.16}$$

$$H_{B_H} = \sum_{j_H=1}^{n} 2\sigma_Z^{[j_H]} \tag{4.17}$$

$$H_{B_L} = \sum_{j_L=1}^{n} 2\sigma_Z^{[j_L]}. \tag{4.18}$$

We also take the external system the discrete infinite dimension system, whose Hamiltonian is

$$H_{E_X} = \sum_{k_{E_X}=-\infty}^{\infty} k_{E_X} |k_{E_X}\rangle\langle k_{E_X}|. \tag{4.19}$$

We assume the initial states of B_H and B_L to be Gibbs states at the temperatures $30K$ and $15K$. For an arbitrary FQSM-work extraction on $SB_HB_LE_X$ whose absorbed heat satisfies $Q_{H,n} = 0.3n^{2/3}$, the efficiency of the FQSM-work extraction is less than the purple line in Fig.4.1.3. On the other hand, there exists a concrete FQSM-work extraction whose efficiency satisfies the blue line in Fig.4.1.3:

$$V_{SB_HB_LE_X} = \sum_{k_{B_H}=1}^{2^n} \sum_{k_S=0}^{1} \sum_{k_{B_L}=1}^{2^n} \sum_{k_{E_X}=-\infty}^{\infty} |f_n(k_{B_H}, k_{B_L}), k_S, g_n(k_{B_H}, k_{B_L}), k_{E_X} + k_{B_H} + k_{B_L} - f_n(k_{B_H}, k_{B_L}) - g_n(k_{B_H}, k_{B_L})\rangle\langle k_{B_H}, k_S, k_{B_L}, k_{E_X}|$$

where $|k_{B_H}\rangle$ and $|k_{B_L}\rangle$ are the k-th energy eigen states of B_H and B_L, and where

$$f_n(k_{B_H}, k_{B_L}) := k_{B_L} - (\lceil k_{B_L} d^{-n+m_n} \rceil - 1)d^{n-m_n} + (\lceil k_{B_H} d^{-m_n} \rceil - 1)d^{m_n} \tag{4.20}$$

$$g_n(k_{B_H}, k_{B_L}) := (k_{B_H} - (\lceil k_{B_H} d^{-m_n} \rceil - 1)d^{m_n} - 1)d^{n-m_n} + \lceil k_{B_L} d^{-n+m_n} \rceil \tag{4.21}$$

$$m_n := \left\lfloor \frac{0.01n^{2/3} + \frac{0.09n^{4/3}}{2n\sigma^2(1/30)}}{\log 2} \right\rfloor \tag{4.22}$$

To see the accuracy of (4.13) as an approximation of $\eta^{(n)}(\{\overline{\mathcal{E}}_j, w_j\})$, we also plot the results of numerical calculation for $\eta^{(n)}(\{\overline{\mathcal{E}}_j, w_j\}) + O(e^{-n\gamma})$ in Fig.4.1.3, where γ is a positive constant value which will be explained

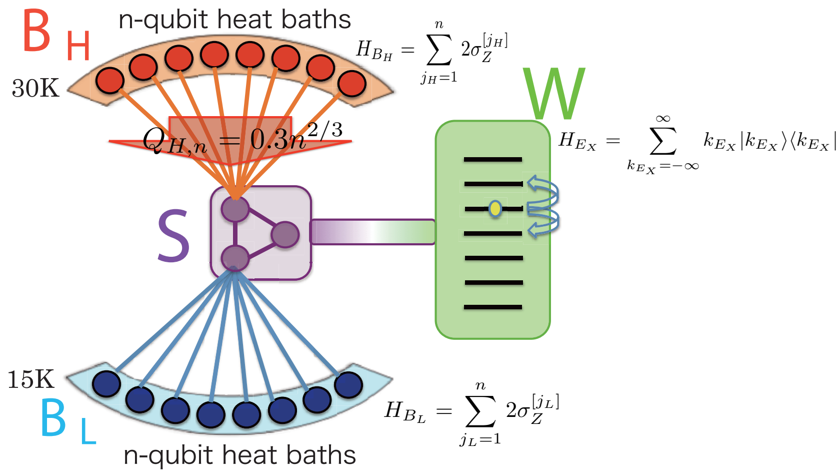

Figure 4.1: qubit engine

in the proof section. Figure 4.1.3 shows that in the scale where the number of particle n is larger than 10^5, the difference between the thermodynamical bound (4.10) and the asymptotic expansion (4.13) of the efficiency $\eta^{(n)}(\{\tilde{\mathcal{E}}_j, w_j\})$ is small. Figure 4.1.3 shows that (4.13) is a very good approximation of $\eta^{(n)}(\{\overline{\mathcal{E}}_j, w_j\})$ for the case $n \geq 6000$. Figure 2 also shows that (4.10) and (4.13) converge to Carnot's bound in the macroscopic limit $n \to \infty$.

4.1.4 Effect of finiteness of the working body

We treat two kinds of finiteness, i.e., the finiteness of heat baths and the finiteness of working body. Now, we discuss which finiteness is essential to decrease the optimal efficiency. In our set up of the n-particle thermodynamic operation, the system (working body) S is composed can be finite with l particles. However, the general upper bound (4.7) is independent of l, and we can perform $\{\overline{\mathcal{E}}_j, w_j\}$ for at least $l \geq 2$ as the two-qubit heat engine. Note that the finiteness of working body may indirectly restrict the optimal efficiency for heat engines. In usual heat engines, only a portion of the total heat baths interacts with working body. The volume of the portion is restricted by the surface area of working body. Thus, the effective number of particles of the heat baths might depend on the surface area of the working body. Such an indirect finite-size effect of the working body might affect the optimal efficiency for a particular model of heat engine. However, as for the direct effect, the efficiency of heat engine is restricted only by the finiteness of heat baths.

4.2 Proof

4.2.1 Rough Sketch

We firstly overview the rough sketch of the proof of our theorems. A rigorous proof is given in the subsections on and after 4.2.2.

General upper bound for efficiency: We derive the upper bound (4.7) in Theorem 4 from the following expressions of $\eta^{(n)}$, which is given by the method of Ref. [8], which was shown in Chapter 3:

$$\eta(\{\mathcal{E}_j, w_j\}) \leq \left(1 - \frac{\beta_H}{\beta_L}\right) - \frac{D(\rho_{\text{fin}}||\rho_{\text{ini}})}{\beta_L Q_{H,n}(\{\mathcal{E}_j, w_j\})}. \tag{4.23}$$

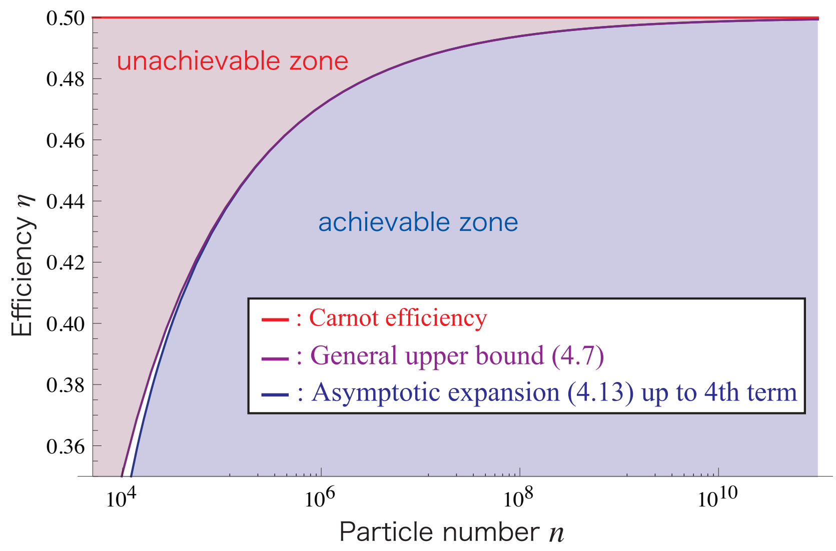

Figure 4.2: We plot Carnot's bound, the thermodynamical upper bound (4.7) and our asymptotic expansion (4.13) up to its fourth term, as the red straight line, the purple curved line and the blue curved line, respectively. The horizontal axis is the number of particles n from 5000 to 10^{11}, and the vertical axis is the efficiency. We put the energy levels of each particle of heat baths to $+k_B J$ and $-k_B J$, and the temperature of heat baths to $30K$ and $15K$, and the extracted heat to $Q_{H,n} = 0.3n^{2/3}k_B J$. The blue region is the achievable zone, while the red region is the unachievable zone.

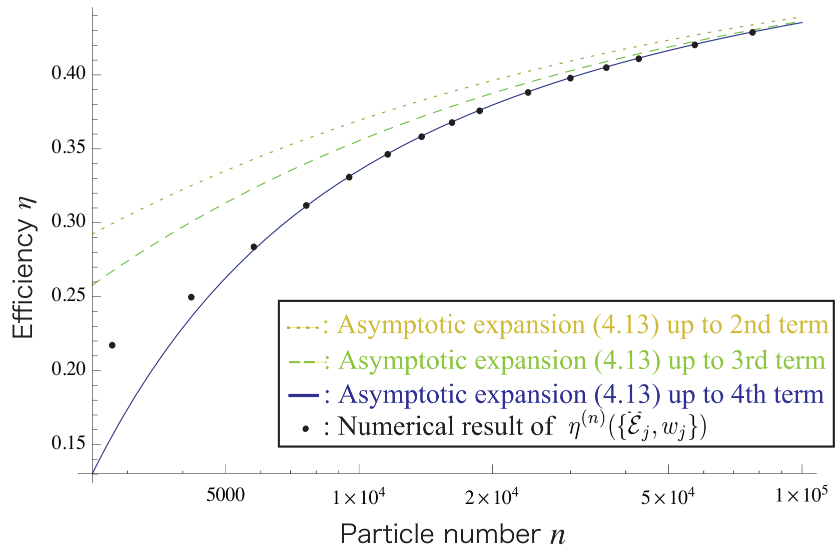

Figure 4.3: We plot the asymptotic expansion (4.7) up to second term, the third term, and the fourth term, as the yellow dotted line, the green broken curve and the blue curve, respectively. We also plot the numerical results of $\eta^{(n)}(\{\mathcal{E}_j, w_j\}) + O(e^{-n\gamma})$ as the black dots. The horizontal axis is the number of particles n from 2500 to 10^5, and the vertical axis is the efficiency. The energy levels, the temperatures of heat baths, and the extracted heat are the same as Fig.4.1.3.

The inequality (4.23) implies that a lower bound of $D(\rho_{\rm fin}||\rho_{\rm ini})$ gives an upper bound of η directly with the fixed extracted heat; $Q_{H,n}(\{\mathcal{E}_j, w_j\}) = Q_H$. Because $\{\mathcal{E}_j, w_j\}$ is the weak work extraction, the transformation $\Lambda(\rho) := \sum_j \mathcal{E}_j(\rho)$ is unital, and thus $S(\rho_{\rm ini}) \le S(\rho_{\rm fin})$ holds. Hence, we minimize $D(\rho_{\rm fin}||\rho_{\rm ini})$ with the constraints $Q_H = {\rm tr}[H_{B_H}(\rho_{\rm ini}^{B_H} - \rho_{\rm fin}^{B_H})]$, $\rho^S_{\rm ini} = \rho^S_{\rm fin}$ and $S(\rho_{\rm ini}) \le S(\rho_{\rm fin})$, and give (4.7) by substituting the minimum for (4.23).

Asymptotic expansion of general upper bound for efficiency: As the former half part of Theorem 5, we derive the inequality (4.10). At first, we asymptotically expand $D(\rho_{{\rm G},\beta'_X}\|\rho_{{\rm G},\beta_X})$ in the terms of $\Delta_X S := S(\beta'_X) - S(\beta_X)$ (X is H or L):

$$D(\rho_{G,\beta'_X}\|\rho_{G,\beta_X}) = \frac{1}{2\beta_X^2\sigma^2(\beta_X)}(\Delta_X S)^2 + (\frac{1}{2\beta_X^4\sigma^4(\beta_X)} + \frac{\gamma_1(\beta_X)}{6\beta_X^3\sigma^3(\beta_X)})(\Delta_X S)^3 + O((\Delta_X S)^4). \quad (4.24)$$

Second, we investigate how $\Delta_H S$ depends on n and $Q_{H,n}$. Solving (4.8), we obtain;

$$\Delta_H S = -\frac{\beta_H Q_H}{n} - \frac{1}{2\beta_H^2\sigma^2(\beta_H)}(\frac{\beta_H Q_H}{n})^2 + O((\frac{\beta_H Q_H}{n})^3). \quad (4.25)$$

We also obtain $\Delta_L S = -\Delta_H S$ from (4.9). Finally, substituting (4.88), (4.25) and $\Delta_L S = -\Delta_H S$ for (4.7), we obtain (4.10).

Classical model: Next, we prove the existence of the CPSU-work extraction which satisfies (4.13). First, note that we have pointed out in the section 3.3 that for an arbitrary classical work extraction, we can take a CPSU-work extraction whose probabilistic distribution of the extracted work is the same as that of the classical work extraction. Thus, in order to show the existence of the CPSU-work extraction which satisfies the equality (4.13), we only have to find a classical work extraction whose efficiency satisfies (4.13).

Let us give the classical work extraction whose efficiency satisfies (4.13). As the set of states of the classical system $\mathcal{X}$, we consider the set of natural numbers $\{j_H, j_L\}$ where $1 \le j_H \le d^n$ and $1 \le j_L \le d^n$. The initial distribution of the classical system $\mathcal{J}$ is $p^{n\downarrow}_{\beta_H}(j_H)p^{n\downarrow}_{\beta_L}(j_L)$, where $p^{n\downarrow}_{\beta_H}(j_H)$ and $p^{n\downarrow}_{\beta_L}(j_L)$ are the descending ordered diagonal elements of $\rho^{\otimes n}_{{\rm G},\beta_H}$ and $\rho^{\otimes n}_{{\rm G},\beta_L}$, respectively. The Hamiltonian of the classical system is $h_H(j_H)+h_L(j_L)$, where $h_H(j_H) := h_H(1) + \frac{1}{\beta_H}\log\frac{p^{n\downarrow}_{\beta_H}(1)}{p^{n\downarrow}_{\beta_H}(j_H)}$ and $h_L(j_L) := h_L(1) + \frac{1}{\beta_L}\log\frac{p^{n\downarrow}_{\beta_L}(1)}{p^{n\downarrow}_{\beta_L}(j_L)}$, and where $h_H(1)$ and $h_L(1)$ are the ground energy of B_H and B_L. Because the classical system and its initial distribution corresponds to $B_H B_L$ and $\rho^{\otimes n}_{{\rm G},\beta_H} \otimes \rho^{\otimes n}_{{\rm G},\beta_L}$, if there is a bi-stochastic matrix $T(j'_H, j'_L|j_H, j_L)$ on $\mathcal{J}$ which satisfies (4.13), then there also exists a CPSU-work extraction on $B_H B_L$ which satisfies (4.13). The bi-stochastic matrix which satisfies (4.13) is given in the following form;

$$\begin{aligned} T_{m_n}(j'_H, j'_L|j_H, j_L) &:= \delta_{j'_H, j_{L1}+(j_{H2}-1)d^{m_n}}\delta_{j'_L,(j_{H1}-1)d^{n-m_n}+j_{L2}}, & (4.26)\\ j_{H2} &:= \lceil j_H d^{-m_n}\rceil, & (4.27)\\ j_{H1} &:= j_H - (j_{H2}-1)d^{m_n} & (4.28)\\ j_{L2} &:= \lceil j_L d^{-n+m_n}\rceil, & (4.29)\\ j_{L1} &:= j_L - (j_{L2}-1)d^{n-m_n}, & (4.30)\end{aligned}$$

where m_n is a natural number. As we will show below, T_{m_n} satisfies (4.13) when $m_n = \left\lfloor \frac{\beta_H n\tilde{q}_n + \frac{n^2\tilde{q}_n^2}{2n\sigma^2(\beta_H)}}{\log d}\right\rfloor$.

Asymptotic expansion of $\eta(T_{m_n})$ In order to show the fact that T_{m_n} satisfies (4.13), we firstly show that the following equality holds;

$$\eta(T_{m_n}) = \left(1 - \frac{\beta_H}{\beta_L}\right) - \frac{D(P_{\text{fin}}^{B_H B_L}||p_{\text{G},\beta_H}^{n\downarrow} p_{\text{G},\beta_L}^{n\downarrow})}{\beta_L Q_{H,n}}, \tag{4.31}$$

where

$$\begin{aligned}
D(P_{\text{fin}}^{B_H B_L}||p_{\text{G},\beta_H}^{n\downarrow} p_{\text{G},\beta_L}^{n\downarrow}) &:= \sum_{j_H, j_L} P_{\text{fin}}^{B_H B_L}(j_H, j_L) \log \frac{P_{\text{fin}}^{B_H B_L}(j_H, j_L)}{p_{\text{G},\beta_H}^{n\downarrow}(j_H) p_{\text{G},\beta_L}^{n\downarrow}(j_L)} && (4.32)\\
\eta(T_{m_n}) &:= \frac{W_{\text{ext}}}{Q_{H,n}} && (4.33)\\
W_{\text{ext}} &:= \sum_{j_H, j_L} (P_{\text{fin}}^{B_H B_L}(j_H, j_L) - p_{\text{G},\beta_H}^{n\downarrow}(j_H) p_{\text{G},\beta_L}^{n\downarrow}(j_L))(h_H(j_H) + h_L(j_L)) && (4.34)\\
Q_{H,n} &:= \sum_{j_H} (P_{\text{fin}}^{B_H}(j_H) - p_{\text{G},\beta_H}^{n\downarrow}(j_H)) h_H(j_H) && (4.35)\\
P_{\text{fin}}^{B_H B_L}(j_H, j_L) &:= \sum_{i_H, i_L} T_{m_n}(j_H, j_L | i_H, i_L) p_{\text{G},\beta_H}^{n\downarrow}(i_H) p_{\text{G},\beta_L}^{n\downarrow}(i_L) && (4.36)\\
P_{\text{fin}}^{B_H}(j_H) &:= \sum_{j_L} P_{\text{fin}}^{B_H B_L}(j_H, j_L). && (4.37)
\end{aligned}$$

The equality (4.31) is given as a special case of (4.23). Because of (4.31), the fact that T_{m_n} satisfies (4.13) will be shown via the asymptotic expansion of the relative entropy $D(P_{\text{fin}}^{B_H B_L}||p_{\text{G},\beta_H}^{n\downarrow} p_{\text{G},\beta_L}^{n\downarrow})$ and the extracted heat $Q_{H,n}$ for T_{m_n}. For the asymptotic expansions of $D(P_{\text{fin}}^{B_H B_L}||p_{\text{G},\beta_H}^{n\downarrow} p_{\text{G},\beta_L}^{n\downarrow})$ and $Q_{H,n}$, we first approximate $D(P_{\text{fin}}^{B_H B_L}||p_{\text{G},\beta_H}^{n\downarrow} p_{\text{G},\beta_L}^{n\downarrow})$ and $Q_{H,n}$ with the relative entropies D_{B_H} and D_{B_L}:

$$\begin{aligned}
D(P_{\text{fin}}^{B_H B_L}||p_{\text{G},\beta_H}^{n\downarrow} p_{\text{G},\beta_L}^{n\downarrow}) &= D_{B_H}(m_n) + D_{B_H}(m_n) + O(e^{-n\alpha_1}) && (4.38)\\
\beta_H Q_{H,n} &= m_n \log d - D_{B_H}(m_n) + O(e^{-n\alpha_2}) && (4.39)
\end{aligned}$$

holds for proper real numbers $\alpha_1 > 0$ and $\alpha_2 > 0$, where

$$D_{B_H}(m_n) := \sum_{j=1}^{d^n} p_{\beta_H}^{n\downarrow}(j) \log \frac{p_{\beta_H}^{n\downarrow}(j)}{d^{-m_n} p_{\beta_H}^{n\downarrow}(\lceil j d^{-m_n} \rceil)} \tag{4.40}$$

$$D_{B_L}(m_n) := \sum_{j=1}^{d^n} p_{\beta_L}^{n\downarrow}(j) \log \frac{p_{\beta_L}^{n\downarrow}(j)}{d^{m_n} p_{\beta_L}^{n\downarrow}(\lceil j d^{m_n} \rceil)} \tag{4.41}$$

where $\lceil x \rceil$ is the ceiling function of x. We can calculate $D_{B_H}(m_n)$ and $D_{B_H}(m_n) + D_{B_L}(m_n)$ with using the strong large deviation theory [46, 47] as follows;

$$\begin{aligned}
D_{B_H}(m_n) &= \frac{(m_n \log d)^2}{n 2 \beta_H^2 \sigma^2(\beta_H)} + O(\frac{m_n^3}{n^2}), && (4.42)\\
D_{B_H}(m_n) + D_{B_L}(m_n) &= c_{\beta_H,\beta_L}^{(1)} \frac{Q_{H,n}^2}{n} - c_{\beta_H,\beta_L}^{(2)} \frac{Q_{H,n}^3}{n^2} + d_{\beta_H,\beta_L}^{(1)} \frac{Q_{H,n}^2}{n^2} + O\left(\frac{Q_{H,n}^3}{n^{5/2}}\right) + O\left(\frac{Q_{H,n}^4}{n^3}\right) && (4.43)
\end{aligned}$$

Then, we obtain (4.13) combining (4.31), (4.38), (4.39), (4.42) and (4.43). Note that if we can directly calculate $D_{B_H}(m_n)$ and $D_{B_L}(m_n)$ precisely, we can obtain an extremely precise approximation of $\eta^{(n)}(T_{m_n})$ whose error is in the order of $O(e^{-n(\alpha_1+\alpha_2)})$. Thus, we obtain the precise values of $D_{B_H}(m_n)$ and $D_{B_L}(m_n)$ by numerous calculation, and plot the extremely precise approximation of $\eta^{(n)}(T_{m_n})$ as the balck dots of Fig. 3.

General method for asymptotic expansion of $\eta(T_{m_n})$: In the derivation of (4.42) and (4.43), we need a high-order asymptotic analysis which have never been used in quantum information. Let us a random variable $Z_X := \log p^{n\downarrow}_{\mathrm{G},\beta_X}(\hat{j}) + nS(\beta_X)$ (X=H or L), where $\hat{j}$ is a random variable on the natural numbers $\{j\}_{j=1}^{d^n}$ that takes the value j with the probability $p^{n\downarrow}_{\mathrm{G},\beta_H}(j)$. We also define the functions $F_X(a)$ and the random variables $\Delta_X Z_X$ as

$$
\begin{aligned}
F_X(a) &:= P_C[Z_X \geq a] &(4.44)\\
F_H(Z_H + \Delta_H Z_H)d^{m_n} &= F_H(Z_H), &(4.45)\\
F_L(Z_L)d^{m_n} &= F_L(Z_L - \Delta_L(Z_L)), &(4.46)
\end{aligned}
$$

where P_C is the counting measure. Then, by definition, the following two equalities hold:

$$
\begin{aligned}
D_{B_H}(m_n) &= E_{\hat{j}}[m_n \log d - \sqrt{n}\Delta_H Z_H] &(4.47)\\
D_{B_L}(m_n) &= E_{\hat{j}}[-m_n \log d + \sqrt{n}\Delta_L Z_L], &(4.48)
\end{aligned}
$$

where $E_{\hat{j}}[...]$ is the expectation value with $\hat{j}$. Thus, we only have to derive $E_{\hat{j}}[\Delta_X Z_X]$. We calculate $E_{\hat{j}}[\Delta_X Z_X]$ by the following three steps. First, we expand $\log F_X(a)$ asymptotically by using strong large deviation theory [46, 47]. Second, we solve (4.136) and (4.137) with using the asymptotic expansion of $\log F_X(a)$, and obtain the asymptotic expansion of $\Delta_X Z_Z$ within $1/\sqrt{n}$, β_X and Z_X. Finally, we obtain the asymptotic expansion of $E_{\hat{j}}[\Delta_X Z_X]$ by calculating $E_{\hat{j}}[Z_X]$. In the the section 4.2 materials, we calculate the asymptotic expansion of $\eta^{(n)}(T_{m_n})$ up to the order of $Q_{H,n}/n^2$ by the above method. However, note that our method is available to calculate the more high orders. With our methods, we can calculate $\eta^{(n)}(T_{m_n})$ with arbitrary accuracy.

4.2.2 Abbrebiations

Hereafter, we will use the following abbreviations for the simplicity:

$$
\rho^S = \mathrm{tr}_{B_H B_L}[\rho],\ \ \rho^{B_H} = \mathrm{tr}_{SB_L}[\rho],\ \ \rho^{B_L} = \mathrm{tr}_{SB_H}[\rho],\ \ \rho^{B_H B_L} = \mathrm{tr}_S[\rho], \tag{4.49}
$$

where ρ is an arbitrary state of the whole system SB_HB_L. As in section 2.1, we will use

$$
\begin{aligned}
-\beta_H H_{B_H} - \mathrm{tr}[\exp(-\beta_H H_{B_H})] &= \log \rho^{B_H}_{\mathrm{ini}}, &(4.50)\\
-\beta_L H_{B_L} - \mathrm{tr}[\exp(-\beta_L H_{B_L})] &= \log \rho^{B_L}_{\mathrm{ini}}. &(4.51)
\end{aligned}
$$

4.2.3 Derivation of the general upper bound

In the present section, we prove Theorem 4;

Theorem 6 (General upper bound for efficiency)**.** *When an n-particle thermodynamic operation $\{\mathcal{E}_j, w_j\}$ has a constant endothermic energy amount Q_H, the efficiency $\eta^{(n)}(\{\mathcal{E}_j, w_j\})$ is bounded as follows;*

$$
\eta^{(n)}(\{\mathcal{E}_j, w_j\}) \leq \left(1 - \frac{\beta_H}{\beta_L}\right) - \frac{n(D(\rho_{\mathrm{G},\beta_H(1+s)}||\rho_{\mathrm{G},\beta_H}) + D(\rho_{\mathrm{G},\beta_L(1-t)}||\rho_{\mathrm{G},\beta_L}))}{\beta_L Q_H} \tag{4.52}
$$

where the real numbers s and t determined by

$$
\begin{aligned}
-\mathrm{tr}\left[\rho_{\mathrm{G},\beta_H(1+s)}\log\rho_{\mathrm{G},\beta_H}\right] &= S(\beta_H)-\frac{\beta_H Q_H}{n}, &(4.53)\\
S(\beta_H(1+s))+S(\beta_L(1-t)) &= S(\beta_H)+S(\beta_L). &(4.54)
\end{aligned}
$$

Proof of Theorem 4 To derive the upper bound (4.52), we employ the following expression of the efficiencies $\eta^{(n)}(\{\mathcal{E}_j, w_j\})$:

$$
\eta^{(n)}(\{\mathcal{E}_j, w_j\}) \quad \le \quad \left(1-\frac{\beta_H}{\beta_L}\right)-\frac{D(\rho_{\mathrm{fin}}||\rho_{\mathrm{ini}})}{\beta_L Q_{H,n}(\{\mathcal{E}_j, w_j\})}, \tag{4.55}
$$

which can derived from the relation $S(\rho_{\mathrm{ini}})\le S(\rho_{\mathrm{fin}})$ by the method in Ref. [8], which is introduced in section 2.1, as follows. Using the relation $S(\rho_{\mathrm{ini}})\le S(\rho_{\mathrm{fin}})$, we have

$$
\begin{aligned}
& -D(\rho_{\mathrm{fin}}\|\rho_{\mathrm{ini}}) \ge -\mathrm{tr}[(\rho_{\mathrm{ini}}-\rho_{\mathrm{fin}})\log\rho_{\mathrm{ini}}]\\
\overset{(a)}{=}\ & -\mathrm{tr}[(\rho_{\mathrm{ini}}^{B_H}-\rho_{\mathrm{fin}}^{B_H})\log\rho_{\mathrm{ini}}^{B_H}]-\mathrm{tr}[(\rho_{\mathrm{ini}}^{B_L}-\rho_{\mathrm{fin}}^{B_L})\log\rho_{\mathrm{ini}}^{B_L}]-\mathrm{tr}[(\rho_{\mathrm{ini}}^{S}-\rho_{\mathrm{fin}}^{S})\log\rho_{\mathrm{ini}}^{S}]\\
\overset{(b)}{=}\ & \beta_H\mathrm{tr}[(\rho_{\mathrm{ini}}^{B_H}-\rho_{\mathrm{fin}}^{B_H})H_{B_H}]+\beta_L\mathrm{tr}[(\rho_{\mathrm{ini}}^{B_L}-\rho_{\mathrm{fin}}^{B_L})H_{B_L}]+\beta_L\mathrm{tr}[(\rho_{\mathrm{ini}}^{S}-\rho_{\mathrm{fin}}^{S})H_S]\\
=\ & (\beta_L+(\beta_H-\beta_L))\mathrm{tr}[(\rho_{\mathrm{ini}}^{B_H}-\rho_{\mathrm{fin}}^{B_H})H_{B_H}]+\beta_L\mathrm{tr}[(\rho_{\mathrm{ini}}^{B_L}-\rho_{\mathrm{fin}}^{B_L})H_{B_L}]+\beta_L\mathrm{tr}[(\rho_{\mathrm{ini}}^{S}-\rho_{\mathrm{fin}}^{S})H_S]\\
\overset{(c)}{=}\ & (\beta_H-\beta_L)Q_{H,n}(\{\mathcal{E}_j, w_j\})+\beta_L W_{\mathrm{ext}}^{(n)}(\{\mathcal{E}_j, w_j\}),
\end{aligned} \tag{4.56}
$$

where (a) follows from $\rho_{\mathrm{ini}}=\rho_{\mathrm{ini}}^{S}\otimes\rho_{\mathrm{ini}}^{B_H}\otimes\rho_{\mathrm{ini}}^{B_L}$, (b) follows from (4.50), (4.51) and $\rho_{\mathrm{ini}}^{S}=\rho_{\mathrm{fin}}^{S}$, (c) follows from (4.4) and (4.5). Therefore, we obtain (4.55) as

$$
\eta^{(n)}(\{\mathcal{E}_j, w_j\})=\frac{W_{\mathrm{ext}}^{(n)}(\{\mathcal{E}_j, w_j\})}{Q_{H,n}(\{\mathcal{E}_j, w_j\})}\le\left(1-\frac{\beta_H}{\beta_L}\right)-\frac{D(\rho_{\mathrm{fin}}||\rho_{\mathrm{ini}})}{\beta_L Q_{H,n}(\{\mathcal{E}_j, w_j\})}. \tag{4.57}
$$

Hence, it is sufficient to prove the inequality

$$
D(\rho_{\mathrm{fin}}||\rho_{\mathrm{ini}})\ge n\left(D(\rho_{\mathrm{G},\beta_H(1+s)}||\rho_{\mathrm{G},\beta_H})+D(\rho_{\mathrm{G},\beta_L(1-t)}||\rho_{\mathrm{G},\beta_L})\right) \tag{4.58}
$$

for any n-particle thermodynamic operation satisfying the constraint $Q_{H,n}(\{\mathcal{E}_j, w_j\})=Q_H$. Because of (4.50), the endothermic energy amount $Q_{H,n}(\{\mathcal{E}_j, w_j\})$ is written as

$$
\begin{aligned}
Q_{H,n}(\{\mathcal{E}_j, w_j\}) &= \mathrm{tr}[H_{B_H}(\rho_{\mathrm{ini}}^{B_H}-\rho_{\mathrm{fin}}^{B_H})]=-\frac{1}{\beta_H}\mathrm{tr}[(\rho_{\mathrm{ini}}^{B_H}-\rho_{\mathrm{fin}}^{B_H})\log\rho_{\mathrm{ini}}^{B_H}]=\frac{1}{\beta_H}\left(S(\rho_{\mathrm{ini}}^{B_H})+\mathrm{tr}[\rho_{\mathrm{fin}}^{B_H}\log\rho_{\mathrm{ini}}^{B_H}]\right)\\
&=\frac{1}{\beta_H}\left(S(\rho_{\mathrm{ini}}^{B_H})-S(\rho_{\mathrm{fin}}^{B_H})+S(\rho_{\mathrm{fin}}^{B_H})+\mathrm{tr}[\rho_{\mathrm{fin}}^{B_H}\log\rho_{\mathrm{ini}}^{B_H}]\right)=\frac{1}{\beta_H}\left(S(\rho_{\mathrm{ini}}^{B_H})-S(\rho_{\mathrm{fin}}^{B_H})-D(\rho_{\mathrm{fin}}^{B_H}\|\rho_{\mathrm{ini}}^{B_H})\right).
\end{aligned} \tag{4.59}
$$

Thus, the constraint $Q_{H,n}(\{\mathcal{E}_j, w_j\})=Q_H$ is equivalent to $Q_H=\frac{1}{\beta_H}\left(S(\rho_{\mathrm{ini}}^{B_H})-S(\rho_{\mathrm{fin}}^{B_H})-D(\rho_{\mathrm{fin}}^{B_H}\|\rho_{\mathrm{ini}}^{B_H})\right)$. Because every n-particle thermodynamic operation is a unital operation, it preserves or increases the entropy of the whole system. Under such entropy-increasing transformations, the relative entropy $D(\rho_{\mathrm{fin}}\|\rho_{\mathrm{ini}})$ is bounded by the following lemma, and thus (4.52) holds for any thermodynamic operation. □

Lemma 9. *For an arbitrary real number* Q_H*,*

$$\min_{\rho}\left\{D(\rho\|\rho_{\rm ini})\middle|S(\rho)\geq S(\rho_{\rm ini}),\ \ \beta_H Q_H = S(\rho_{\rm ini}^{B_H}) - S(\rho^{B_H}) - D(\rho^{B_H}\|\rho_{\rm ini}^{B_H}),\ \ \rho_{\rm ini}^{S}=\rho^{S}\right\}$$
$$= n\left(D(\rho_{{\rm G},\beta_H(1+s)}||\rho_{{\rm G},\beta_H}) + D(\rho_{{\rm G},\beta_L(1-t)}||\rho_{{\rm G},\beta_L})\right) \tag{4.60}$$

holds, where the real numbers s *and* t *determined by* (4.53) *and* (4.54)*.*

To show Lemma 1, we prepare the following lemma:

Lemma 10. *For a given state* ρ *and a real number* $C>0$*,*

$$\min_{\rho':S(\rho')\geq C} -{\rm tr}[\rho'\log\rho] = -{\rm tr}\left[\frac{\rho^{1-x}}{{\rm tr}[\rho^{1-x}]}\log\rho\right], \tag{4.61}$$

where x *is a real number satisfying that*

$$S\left(\frac{\rho^{1-x}}{{\rm tr}[\rho^{1-x}]}\right) = C \tag{4.62}$$

Proof of Lemma 2:

$$\begin{aligned}
{\rm tr}\left[\frac{\rho^{1-x}}{{\rm tr}[\rho^{1-{\rm x}}]}\log\rho\right] - {\rm tr}[\rho'\log\rho] &= {\rm tr}\left[\left(\frac{\rho^{1-x}}{{\rm tr}[\rho^{1-{\rm x}}]}-\rho'\right)\log\rho\right] = \frac{1}{1-x}{\rm tr}\left[\left(\frac{\rho^{1-x}}{{\rm tr}[\rho^{1-{\rm x}}]}-\rho'\right)\log\frac{\rho^{1-x}}{{\rm tr}[\rho^{1-{\rm x}}]}\right]\\
&= \frac{1}{1-x}\left(-S(\frac{\rho^{1-x}}{{\rm tr}[\rho^{1-{\rm x}}]}) + S(\rho') + D\left(\rho'\|\frac{\rho^{1-x}}{{\rm tr}[\rho^{1-{\rm x}}]}\right)\right)\\
&= \frac{1}{1-x}\left(S(\rho') - C + D\left(\rho'\|\frac{\rho^{1-x}}{{\rm tr}[\rho^{1-{\rm x}}]}\right)\right)\geq 0. \qquad (4.63)
\end{aligned}$$

The equality is valid only when $S(\rho')=C$ and $\rho'=\frac{\rho^{1-x}}{{\rm tr}[\rho^{1-{\rm x}}]}$ hold. □

Proof of Lemma 1: Firstly, we point out that the $\rho_{\rm min} := \rho_{\rm G,\beta_H(1+s)}^{\otimes n}\otimes\rho_{\rm ini}^{S}\otimes\rho_{{\rm G},\beta_{\rm L}(1-{\rm t})}^{\otimes n}$ satisfies the conditions $S(\rho)\geq S(\rho_{\rm ini})$, $\beta_H Q_H = S(\rho_{\rm ini}^{B_H}) - S(\rho_{\rm fin}^{B_H}) - D(\rho^{B_H}\|\rho_{\rm ini}^{B_H})$ and $\rho_{\rm ini}^{S}=\rho^{S}$, and satisfies

$$D(\rho_{\rm min}\|\rho_{\rm ini}^{B_H B_L}) = n\left(D(\rho_{{\rm G},\beta_H(1+s)}||\rho_{{\rm G},\beta_H}) + D(\rho_{{\rm G},\beta_L(1-t)}||\rho_{{\rm G},\beta_L})\right). \tag{4.64}$$

Thus, we only have to prove

$$\min_{\rho}\left\{D(\rho\|\rho_{\rm ini})\middle|S(\rho)\geq S(\rho_{\rm ini}),\ \ \beta_H Q_H = S(\rho_{\rm ini}^{B_H}) - S(\rho^{B_H}) - D(\rho^{B_H}\|\rho_{\rm ini}^{B_H}),\ \ \rho_{\rm ini}^{S}=\rho^{S}\right\}$$
$$\leq n\left(D(\rho_{{\rm G},\beta_H(1+s)}||\rho_{{\rm G},\beta_H}) + D(\rho_{{\rm G},\beta_L(1-t)}||\rho_{{\rm G},\beta_L})\right). \tag{4.65}$$

Under the given constraints, we can convert $D(\rho\|\rho_{\rm ini})$ as follows;

$$\begin{aligned}
D(\rho\|\rho_{\rm ini}) &\overset{(a)}{=} -S(\rho) - {\rm tr}[\rho^S\log\rho_{\rm ini}^S] - {\rm tr}[\rho^{B_H}\log\rho_{\rm ini}^{B_H}] - {\rm tr}[\rho^{B_L}\log\rho_{\rm ini}^{B_L}]\\
&\overset{(b)}{\leq} -S(\rho_{\rm ini}^{B_H}) - S(\rho_{\rm ini}^{B_L}) - {\rm tr}[\rho^{B_H}\log\rho_{\rm ini}^{B_H}] - {\rm tr}[\rho^{B_L}\log\rho_{\rm ini}^{B_L}] \qquad (4.66)\\
&= -S(\rho_{\rm ini}^{B_L}) - S(\rho_{\rm ini}^{B_H}) + D(\rho^{B_H}\|\rho_{\rm ini}^{B_H}) + S(\rho_{\rm ini}^{B_H}) - {\rm tr}[\rho^{B_L}\log\rho_{\rm ini}^{B_L}]\\
&\overset{(c)}{=} -S(\rho_{\rm ini}^{B_L}) - \beta_H Q_H - {\rm tr}[\rho^{B_L}\log\rho_{\rm ini}^{B_L}] \qquad (4.67)\\
&\overset{(d)}{=} n\left(D(\rho_{{\rm G},\beta_H(1+s)}||\rho_{{\rm G},\beta_H}) + D(\rho_{{\rm G},\beta_L(1-t)}||\rho_{{\rm G},\beta_L})\right)\\
&\quad +{\rm tr}[\rho_{{\rm G},\beta_L(1-t)}^{\otimes n}\log\rho_{\rm ini}^{B_L}] - {\rm tr}[\rho^{B_L}\log\rho_{\rm ini}^{B_L}] \qquad (4.68)
\end{aligned}$$

where (a) follows from $\rho_{\text{ini}} = \rho_{\text{ini}}^S \otimes \rho_{\text{ini}}^{B_H} \otimes \rho_{\text{ini}}^{B_L}$, (b) follows from $S(\rho_{\text{ini}}) \leq S(\rho)$ and $\rho_{\text{ini}}^S = \rho^S$, (c) follows from $\beta_H Q_H = S(\rho_{\text{ini}}^{B_H}) - S(\rho^{B_H}) - D(\rho^{B_H} \| \rho_{\text{ini}}^{B_H})$, (d) follows from (4.53) and (4.54) Thus, in order to prove Lemma 9, it is sufficient to show

$$\operatorname{tr}[\rho_{\mathrm{G},\beta_L(1-t)}^{\otimes n} \log \rho_{\text{ini}}^{B_L}] \leq \operatorname{tr}[\rho^{B_L} \log \rho_{\text{ini}}^{B_L}] \tag{4.69}$$

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

$$S(\rho^{B_L}) \geq S\left(\frac{(\rho_{\text{ini}}^{B_L})^{(1-t)}}{\operatorname{tr}[(\rho_{\text{ini}}^{B_L})^{(1-t)}]}\right). \tag{4.70}$$

Hence, by substituting ρ^{B_L} and $S\left(\frac{(\rho_{\text{ini}}^{B_L})^{(1-t)}}{\operatorname{tr}[(\rho_{\text{ini}}^{B_L})^{(1-t)}]}\right)$ for ρ' and C of Lemma 2, (4.70) guarantees (4.69)

Finally, let us prove (4.70). We have

$$\begin{aligned}
& S(\rho^{B_H}) - S\left(\frac{(\rho_{\text{ini}}^{B_H})^{(1+s)}}{\operatorname{tr}[(\rho_{\text{ini}}^{B_H})^{(1+s)}]}\right) \\
= & -\operatorname{tr}[\rho^{B_H} \log \rho^{B_H}] + \operatorname{tr}\left[\frac{(\rho_{\text{ini}}^{B_H})^{(1+s)}}{\operatorname{tr}[(\rho_{\text{ini}}^{B_H})^{(1+s)}]} \log \frac{(\rho_{\text{ini}}^{B_H})^{(1+s)}}{\operatorname{tr}[(\rho_{\text{ini}}^{B_H})^{(1+s)}]}\right] \\
= & -\operatorname{tr}[\rho^{B_H} \log \rho^{B_H}] + \operatorname{tr}\left[\rho^{B_H} \log \frac{(\rho_{\text{ini}}^{B_H})^{(1+s)}}{\operatorname{tr}[(\rho_{\text{ini}}^{B_H})^{(1+s)}]}\right] + \operatorname{tr}\left[\left(\frac{(\rho_{\text{ini}}^{B_H})^{(1+s)}}{\operatorname{tr}[(\rho_{\text{ini}}^{B_H})^{(1+s)}]} - \rho^{B_H}\right) \log \frac{(\rho_{\text{ini}}^{B_H})^{(1+s)}}{\operatorname{tr}[(\rho_{\text{ini}}^{B_H})^{(1+s)}]}\right] \\
= & -D\left(\rho^{B_H} \Big\| \frac{(\rho_{\text{ini}}^{B_H})^{(1+s)}}{\operatorname{tr}[(\rho_{\text{ini}}^{B_H})^{(1+s)}]}\right) + \operatorname{tr}\left[\left(\frac{(\rho_{\text{ini}}^{B_H})^{(1+s)}}{\operatorname{tr}[(\rho_{\text{ini}}^{B_H})^{(1+s)}]} - \rho^{B_H}\right) \log \frac{(\rho_{\text{ini}}^{B_H})^{(1+s)}}{\operatorname{tr}[(\rho_{\text{ini}}^{B_H})^{(1+s)}]}\right] \\
= & -D\left(\rho^{B_H} \Big\| \frac{(\rho_{\text{ini}}^{B_H})^{(1+s)}}{\operatorname{tr}[(\rho_{\text{ini}}^{B_H})^{(1+s)}]}\right) + (1+s)\operatorname{tr}\left[\left(\frac{(\rho_{\text{ini}}^{B_H})^{(1+s)}}{\operatorname{tr}[(\rho_{\text{ini}}^{B_H})^{(1+s)}]} - \rho^{B_H}\right) \log \rho_{\text{ini}}^{B_H}\right] & (4.71) \\
= & -D\left(\rho^{B_H} \Big\| \frac{(\rho_{\text{ini}}^{B_H})^{(1+s)}}{\operatorname{tr}[(\rho_{\text{ini}}^{B_H})^{(1+s)}]}\right) + (1+s)(-nS(\beta_H) + \beta_H Q_H + S(\rho_{\text{ini}}^{B_H}) - \beta_H Q_H) & (4.72) \\
= & -D\left(\rho^{B_H} \Big\| \frac{(\rho_{\text{ini}}^{B_H})^{(1+s)}}{\operatorname{tr}[(\rho_{\text{ini}}^{B_H})^{(1+s)}]}\right) \leq 0, & (4.73)
\end{aligned}$$

where we use (4.53) and the relation $S(\rho_{\text{ini}}^{B_H}) + \operatorname{tr}\rho^{B_H} \log \rho_{\text{ini}}^{B_H} = \beta_H Q_H$ given from (4.59) to convert (4.71) into (4.72). The subadditivity of the von Neumann entropy, $S(\rho_{\text{ini}}) \leq S(\rho)$ and $\rho_{\text{ini}}^S = \rho^S$ imply

$$S(\rho^{B_H}) + S(\rho^{B_L}) \geq S(\rho_{\text{ini}}^{B_H}) + S(\rho_{\text{ini}}^{B_L}). \tag{4.74}$$

Thus, the combination of (4.54), (4.73), and (4.74) derives (4.70) as follows:

$$S(\rho^{B_L}) \geq -S(\rho^{B_H}) + S(\rho_{\text{ini}}^{B_H}) + S(\rho_{\text{ini}}^{B_L}) \geq -S\left(\frac{(\rho_{\text{ini}}^{B_H})^{(1+s)}}{\operatorname{tr}[(\rho_{\text{ini}}^{B_H})^{(1+s)}]}\right) + S(\rho_{\text{ini}}^{B_H}) + S(\rho_{\text{ini}}^{B_L}) = S\left(\frac{(\rho_{\text{ini}}^{B_L})^{(1-t)}}{\operatorname{tr}[(\rho_{\text{ini}}^{B_L})^{(1-t)}]}\right), \tag{4.75}$$

where s and t are defined in (4.53) and (4.54). □

4.2.4 Relation with cumulant generating function

In the subsection 4.2.3, we have derived a general upper bound (4.7). Next, we asymptotically expand it, and gives (4.10). In the present subsection, we prepare for the derivation of the asymptotic expansion.

Let us introduce the cumulant generating functions $\phi_X(1+s) := \log \operatorname{tr}\rho_{G,\beta_X}^{1+s}$ for $X = H, L$. Then, the variance and the skewness of energy

$$\sigma^2(\beta_X) := \mathrm{tr}[\rho_{\beta_X}(H_{B_X} - \mathrm{tr}[\rho_{\beta_X} H_{B_X}])^2] \tag{4.76}$$

$$\gamma_1(\beta_X) := \frac{\mathrm{tr}[\rho_{\beta_X}(H_{B_X} - \mathrm{tr}[\rho_{\beta_X} H_{B_X}])^3]}{\sigma^3(\beta)} \tag{4.77}$$

satisfies

$$\phi_X''(1) = \beta_X^2 \sigma^2(\beta_X) \tag{4.78}$$

$$\phi_X'''(1) = \beta_X^3 \gamma_1(\beta_X)\sigma^3(\beta_X). \tag{4.79}$$

Note that the Fisher information of the family $\{\rho_{G,\beta_X(1+s)}\}_s$ is $\phi_X''(1+s)$ [59]. The relative entropy and the entropy are written as [59]

$$D(\rho_{G,\beta_X(1+s)}\|\rho_{G,\beta_X}) = \phi_X'(1+s)s - \phi_X(1+s) \tag{4.80}$$

$$S(\beta_X(1+s)) = -(1+s)\phi_X'(1+s) + \phi_X(1+s) = -\phi_X'(1+s) - D(\rho_{G,\beta_X(1+s)}\|\rho_{G,\beta_X}). \tag{4.81}$$

Since ϕ_X is strictly convex, we can define the inverse function of ϕ_X', which is denoted by ψ_X. In the following, we focus on the entropy $S(\beta_X)$, which is denoted by S_X. Then, we have

$$\psi_X'(-S_X) = \phi_X''(1)^{-1} = \frac{1}{\beta_X^2\sigma^2(\beta_X)} \tag{4.82}$$

$$\psi_X''(-S_X) = -\phi_X'''(1)\phi_X''(1)^{-3} = -\frac{\gamma_1(\beta_X)}{\beta_X^3\sigma^3(\beta_X)}. \tag{4.83}$$

When s is close to 0, $A := \phi_X'(1+s)$ is also close to $-S_X$. Hence,

$$\begin{aligned} D(\rho_{G,\beta_X(1+s)}\|\rho_{G,\beta_X}) =& \phi_X'(1+s) - \phi_X(1+s) = \phi_X'(1+s)(\psi_X(A)-1) - \phi_X(\psi_X(A)) \\ =& (\psi_X(-S_X)-1)(A+S_X) + \frac{1}{2}\psi_X'(-S_X)(A+S_X)^2 + \frac{1}{6}\psi_X''(-S_X)(A+S_X)^3 + O((A+S_X)^4) \\ =& \frac{1}{2}\psi_X'(-S_X)(A+S_X)^2 + \frac{1}{6}\psi_X''(-S_X)(A+S_X)^3 + O((A+S_X)^4). \end{aligned} \tag{4.84}$$

Then, the entropy is characterized as

$$S(\beta_X(1+s)) = -\phi_X'(1+s) - D(\rho_{G,\beta_X(1+s)}\|\rho_{G,\beta_X}) = -A - \frac{1}{2}\psi_X'(-S_X)(A+S_X)^2 + O((A+S_X)^3). \tag{4.85}$$

Thus, $\Delta_X S := S(\beta_X(1+s)) - S_X$ satisfies

$$\Delta_X S = -(A+S_X) - \frac{1}{2}\psi_X'(-S_X)(A+S_X)^2 + O((A+S_X)^3), \tag{4.86}$$

which implies

$$-(A+S_X) = \Delta_X S + \frac{1}{2}\psi_X'(-S_X)(\Delta_X S)^2 + O((\Delta_X S)^3). \tag{4.87}$$

Thus,

$$\begin{aligned} D(\rho_{G,\beta_X(1+s)}\|\rho_{G,\beta_X}) =& \frac{1}{2}\psi'_X(-S_X)(\Delta_X S)^2 + (\frac{1}{2}\psi'_X(-S_X)^2 - \frac{1}{6}\psi''_X(-S_X))(\Delta_X S)^3 + O((\Delta_X S)^4) \\ =& \frac{1}{2\beta_X^2\sigma^2(\beta_X)}(\Delta_X S)^2 + (\frac{1}{2\beta_X^4\sigma^4(\beta_X)} + \frac{\gamma_1(\beta_X)}{6\beta_X^3\sigma^3(\beta_X)})(\Delta_X S)^3 + O((\Delta_X S)^4). \end{aligned} \tag{4.88}$$

This relation will be used in the following sections.

4.2.5 Taylor expansion of the general upper bound

Now, we have completed the preparation. Hereafter, we derive the asymptotic expansion (4.10) in the present section, and prove that the classical work extraction T_{m_n} satisfies (4.13) when $m_n = \left\lfloor \frac{\beta_H n\tilde{q}_n + \frac{n^2\tilde{q}_n^2}{2n\sigma^2(\beta_H)}}{\log d} \right\rfloor$ in the next subsection 4.2.6. Namely, in the present subsection and the next subsection 4.2.6, we prove the extended Carnot's Theorem. For the convenience to read, we write down the theorem again;

Theorem 7 (Extended Carnot's Theorem)**.** *When n-particle thermodynamic operations $\{\{\mathcal{E}_j, w_j\}\}_{n=1}^\infty$ have extracted heats $\{Q_{H,n}\}_{n=1}^\infty$ satisfying $\lim_{n\to\infty} Q_{H,n}/n = 0$, the upper bound (4.7) has an asymptotic expansion as follows:*

$$\eta^{(n)}(\{\mathcal{E}_j, w_j\}) \le \left(1 - \frac{\beta_H}{\beta_L}\right) - \sum_{k=1}^{\infty} c_{\beta_H}^{(k)} q_n^k, \tag{4.89}$$

where $q_n := Q_{H,n}/n$ and

$$c_{\beta_H,\beta_L}^{(1)} := \left(\frac{1}{2\beta_H^2\sigma^2(\beta_H)} + \frac{1}{2\beta_L^2\sigma^2(\beta_L)}\right)\frac{\beta_H^2}{\beta_L} \tag{4.90}$$

$$c_{\beta_H,\beta_L}^{(2)} := \left(-\frac{\gamma_1(\beta_H)}{6\beta_H^3\sigma^3(\beta_H)} + \frac{\gamma_1(\beta_L)}{6\beta_L^3\sigma^3(\beta_L)} + \frac{1}{2\beta_L^4\sigma^4(\beta_L)} + \frac{1}{2\beta_H^2\beta_L^2\sigma^2(\beta_H)\sigma^2(\beta_L)}\right)\frac{\beta_H^3}{\beta_L}. \tag{4.91}$$

On the other hand, for an arbitrary sequence of real numbers $\{\tilde{q}_n\}$ which satisfy $\tilde{q}_n \to 0$ at the limit $n \to \infty$, we can take the n-particle thermodynamic operations $\{\overline{\mathcal{E}}_j, w_j\}$ whose extracted heats $\{Q_{H,n}\}$ satisfy $\frac{q_n}{\tilde{q}_n} := \frac{Q_{H,n}}{n\tilde{q}_n} \to 1$ at the limit $n \to \infty$ and

$$\eta^{(n)}(\{\overline{\mathcal{E}}_j, w_j\}) = \left(1 - \frac{\beta_H}{\beta_L}\right) - c_{\beta_H,\beta_L}^{(1)} q_n - c_{\beta_H,\beta_L}^{(2)} q_n^2 - d_{\beta_H,\beta_L}^{(1)} \frac{q_n}{n} + O\left(\frac{q_n^2}{\sqrt{n}}\right) + O\left(q_n^3\right), \tag{4.92}$$

where

$$d_{\beta_H,\beta_L}^{(1)} := \left((\frac{\gamma_1(\beta_H)}{2\beta_H\sigma(\beta_H)} + \frac{1}{\beta_H^2\sigma^2(\beta_H)})^2 + (\frac{\gamma_1(\beta_L)}{2\beta_L\sigma(\beta_L)} + \frac{1}{\beta_L^2\sigma^2(\beta_L)})^2\right)\frac{\beta_H^2}{\beta_L}. \tag{4.93}$$

In the present subsection, we will derive (4.89).

Proof of (4.89)**:** To show (4.89), we employ the notation given in Section 4.2.4. Now, we choose s and t satisfying (4.53) and (4.54). We choose $\Delta_H S$ and $\Delta_L S$ as $\Delta_H S := S(\beta_H(1+s)) - S_H$ and $\Delta_L S := S(\beta_L(1-$

$t)) - S_L$. Thus, the relations (4.53), (4.88), and (4.54) yield that

$$-\frac{\beta_H Q_H}{n} = \Delta_H S + D(\rho_{G,\beta_H s}\|\rho_{G,\beta_H}) = \Delta_H S + \frac{1}{2\beta_H^2\sigma^2(\beta_H)}(\Delta_H S)^2 + O((\Delta_H S)^3) \tag{4.94}$$

$$\Delta_L S = -\Delta_H S. \tag{4.95}$$

Thus,

$$\Delta_H S = -\frac{\beta_H Q_H}{n} - \frac{1}{2\beta_H^2\sigma^2(\beta_H)}(\frac{\beta_H Q_H}{n})^2 + O((\frac{\beta_H Q_H}{n})^3), \tag{4.96}$$

which implies that

$$\Delta_H S^2 =(\frac{\beta_H Q_H}{n})^2 + \frac{1}{\beta_H^2\sigma^2(\beta_H)}(\frac{\beta_H Q_H}{n})^3 + O((\frac{\beta_H Q_H}{n})^4) \tag{4.97}$$

$$\Delta_H S^3 = -(\frac{\beta_H Q_H}{n})^3 + O((\frac{\beta_H Q_H}{n})^4. \tag{4.98}$$

Therefore,

$$\begin{aligned}
& n(D(\rho_{\mathrm{G},\beta_H(1+s)}||\rho_{\mathrm{G},\beta_H}) + D(\rho_{\mathrm{G},\beta_L(1-t)}||\rho_{\mathrm{G},\beta_L})) \\
=& \frac{1}{2\beta_H^2\sigma^2(\beta_H)}(\Delta_H S)^2 + (\frac{1}{2\beta_H^4\sigma^4(\beta_H)} + \frac{\gamma_1(\beta_H)}{6\beta_H^3\sigma^3(\beta_H)})(\Delta_H S)^3 \\
& + \frac{1}{2\beta_L^2\sigma^2(\beta_L)}(\Delta_L S)^2 + (\frac{1}{2\beta_L^4\sigma^4(\beta_L)} + \frac{\gamma_1(\beta_L)}{6\beta_L^3\sigma^3(\beta_L)})(\Delta_L S)^3 + O((\Delta_H S)^4) \\
=& (\frac{1}{2\beta_H^2\sigma^2(\beta_H)} + \frac{1}{2\beta_L^2\sigma^2(\beta_L)})(\Delta_H S)^2 + (\frac{1}{2\beta_H^4\sigma^4(\beta_H)} - \frac{1}{2\beta_L^4\sigma^4(\beta_L)} + \frac{\gamma_1(\beta_H)}{6\beta_H^3\sigma^3(\beta_H)} - \frac{\gamma_1(\beta_L)}{6\beta_L^3\sigma^3(\beta_L)})(\Delta_H S)^3 + O((\Delta_H S)^4) \\
=& (\frac{1}{2\beta_H^2\sigma^2(\beta_H)} + \frac{1}{2\beta_L^2\sigma^2(\beta_L)})(\frac{\beta_H Q_H}{n})^2 \\
& + (-\frac{\gamma_1(\beta_H)}{6\beta_H^3\sigma^3(\beta_H)} + \frac{\gamma_1(\beta_L)}{6\beta_L^3\sigma^3(\beta_L)} + \frac{1}{2\beta_H^2\beta_L^2\sigma^2(\beta_H)\sigma^2(\beta_L)} + \frac{1}{2\beta_L^4\sigma^4(\beta_L)})(\frac{\beta_H Q_H}{n})^3 + O((\Delta_H S)^4).
\end{aligned} \tag{4.99}$$

Therefore, substituting (4.99) into (4.52), we obtain (4.89).

4.2.6 Asymptotic expansion of efficiency $\eta^{(n)}(T_{m_n})$

Here, we prove that $\eta^{(n)}(T_{m_n})$ satisfies (4.92), when $m_n = \left\lfloor \frac{\beta_H n\tilde{q}_n + \frac{n^2\tilde{q}_n^2}{2n\sigma^2(\beta_H)}}{\log d} \right\rfloor$. This is the final part of the proof of Refined Carnot's Theorem. We first derive (4.31), and second derive (4.38) and (4.39), and finally prove (4.42) and (4.43).

4.2.6.1 Derivation of (4.31)

Let us derive (4.31). Because of the definition of the bi-stochasitic matrix $T_{m_n}(j_H', j_L'|j_H, j_L)$, it preserves the entropy; $S(P_{\mathrm{fin}}^{B_H B_L}) = S(p_{\mathrm{G},\beta_H}^{n\downarrow} p_{\mathrm{G},\beta_L}^{n\downarrow})$. Similarly as (4.23), using the relation $S(P_{\mathrm{fin}}^{B_H B_L}) = S(p_{\mathrm{G},\beta_H}^{n\downarrow} p_{\mathrm{G},\beta_L}^{n\downarrow})$, we have

$$
\begin{aligned}
& -D(P_{\text{fin}}^{B_H B_L} \| p_{\text{G},\beta_H}^{n\downarrow} p_{\text{G},\beta_L}^{n\downarrow}) = -\sum_{j_H, j_L} [(p_{\text{G},\beta_H}^{n\downarrow}(j_H) p_{\text{G},\beta_L}^{n\downarrow}(j_L) - P_{\text{fin}}^{B_H, B_L}(j_H, j_L)) \log p_{\text{G},\beta_H}^{n\downarrow}(j_H) p_{\text{G},\beta_L}^{n\downarrow}(j_L)] \\
= & -\sum_{j_H} [(p_{\text{G},\beta_H}^{n\downarrow}(j_H) - P_{\text{fin}}^{B_H}(j_H)) \log p_{\text{G},\beta_H}^{n\downarrow}(j_H)] - \sum_{j_L} [(p_{\text{G},\beta_L}^{n\downarrow}(j_L) - P_{\text{fin}}^{B_L}(j_L)) \log p_{\text{G},\beta_L}^{n\downarrow}(j_L)] \\
= & \beta_H \sum_{j_H} [(p_{\text{G},\beta_H}^{n\downarrow}(j_H) - P_{\text{fin}}^{B_H}(j_H)) h_H(j_H)] + \beta_L \sum_{j_L} [(p_{\text{G},\beta_L}^{n\downarrow}(j_L) - P_{\text{fin}}^{B_L}(j_L)) h_L(j_L)] \\
= & (\beta_L + (\beta_H - \beta_L)) \sum_{j_H} [(p_{\text{G},\beta_H}^{n\downarrow}(j_H) - P_{\text{fin}}^{B_H}(j_H)) h_H(j_H)] + \beta_L \sum_{j_L} [(p_{\text{G},\beta_L}^{n\downarrow}(j_L) - P_{\text{fin}}^{B_L}(j_L)) h_L(j_L)] \\
= & (\beta_H - \beta_L) Q_{H,n} + \beta_L W_{\text{ext}}^{(n)}. \qquad (4.100)
\end{aligned}
$$

Therefore, we obtain (4.31) as

$$
\eta^{(n)}(T_{m_n}) = \frac{W_{\text{ext}}^{(n)}}{Q_{H,n}} = \left(1 - \frac{\beta_H}{\beta_L}\right) - \frac{D(P_{\text{fin}}^{B_H B_L} || p_{\text{G},\beta_H}^{n\downarrow} p_{\text{G},\beta_L}^{n\downarrow})}{\beta_L Q_{H,n}}. \qquad (4.101)
$$

□

Due to (4.31), in order to obtain the asymptotic expansion of $\eta^{(n)}(T_{m_n})$, it is enough to asymptotically expand the relative entropy $D(P_{\text{fin}}^{B_H B_L} || p_{\text{G},\beta_H}^{n\downarrow} p_{\text{G},\beta_L}^{n\downarrow})$ and the endothermic amount $Q_{H,n}$.

4.2.6.2 Approximations of $D(P_{\text{fin}}^{B_H B_L} || p_{\text{G},\beta_H}^{n\downarrow} p_{\text{G},\beta_L}^{n\downarrow})$ and $Q_{H,n}$

Let us prove (4.38) and (4.39). As a preparation for the proof, we introduce the probabilities $\tilde{P}_{\text{fin}}^{B_H}(j_H)$ and $\tilde{P}_{\text{fin}}^{B_L}(j_L)$, whose product $\tilde{P}_{\text{fin}}^{B_H}(j_H) \tilde{P}_{\text{fin}}^{B_L}(j_L)$ approximates the final distribution $P_{\text{fin}}^{B_H B_L}(j_H, j_L)$:

$$
\begin{aligned}
\tilde{P}_{\text{fin}}^{B_H}(j_H) &:= d^{m_n} p_{\text{G},\beta_H}^{n\downarrow}(j_{H2} d^{m_n}) \delta_{j_{H1},1}, \qquad (4.102) \\
\tilde{P}_{\text{fin}}^{B_L}(j_L) &:= d^{-m_n} p_{\text{G},\beta_L}^{n\downarrow}(j_{L2}), \qquad (4.103)
\end{aligned}
$$

where j_{H1}, j_{H2} and j_{L2} are defined as (4.28), (4.27) and (4.29).

First of all, let us show that the probability $\tilde{P}_{\text{fin}}^{B_H} \tilde{P}_{\text{fin}}^{B_L}$ approximates the true probability $P_{\text{fin}}^{B_H B_L}$.

Lemma 11. *When a sequence $\{m_n\}$ satisfies*

$$
m_n < n \left(\min \left\{ 1 - \frac{S(p_{\text{G},\beta_L})}{\log d}, \ -\frac{\log \max_j \{p_{\beta_H}(j)\}_{j=1}^d}{\log d} \right\} - \epsilon \right) \qquad (4.104)
$$

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

$$
\|P_{\text{fin}}^{B_H B_L} - \tilde{P}_{\text{fin}}^{B_H} \tilde{P}_{\text{fin}}^{B_L}\|_1 = O(e^{-n\alpha_1}), \qquad (4.105)
$$

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

Proof: We have

$$\|P_{\rm fin}^{B_H B_L} - \tilde{P}_{\rm fin}^{B_H} \tilde{P}_{\rm fin}^{B_L}\|_1 \tag{4.106}$$
$$= \left| \sum_{j_{H1}, j_{H2}, j_{L1}, j_{L2}} p_{\beta_H}^{n\downarrow}(j_{L1} + (j_{H2}-1)d^{m_n}) p_{\beta_L}^{n\downarrow}(j_{L2} + (j_{H1}-1)d^{n-m_n}) - p_{\beta_H}^{n\downarrow}(j_{H2} d^{m_n}) p_{\beta_L}^{n\downarrow}(j_{L2}) \delta_{1,j_{H1}} \right|$$
$$= \sum_{j_{H2}, j_{L1}, j_{L2}} \left(p_{\beta_H}^{n\downarrow}(j_{L1} + (j_{H2}-1)d^{m_n}) p_{\beta_L}^{n\downarrow}(j_{L2}) - p_{\beta_H}^{n\downarrow}(j_{H2} d^{m_n}) p_{\beta_L}^{n\downarrow}(j_{L2}) \right) \tag{4.107}$$
$$+ \sum_{j_{H1}=2}^{d^{m_n}} \sum_{j_{H2}, j_{L1}, j_{L2}} p_{\beta_H}^{n\downarrow}(j_{L1} + (j_{H2}-1)d^{m_n}) p_{\beta_L}^{n\downarrow}(j_{L2} + (j_{H1}-1)d^{n-m_n}) \tag{4.108}$$
$$\le \sum_{j_{H2}=1}^{d^{n-m_n}} \sum_{j_{L1}=1}^{d^{m_n}} \left(p_{\beta_H}^{n\downarrow}(j_{L1} + (j_{H2}-1)d^{m_n}) - p_{\beta_H}^{n\downarrow}(j_{H2} d^{m_n}) \right) + \sum_{j=1}^{d^n} \sum_{j'=d^{n-m_n}+1}^{d^n} p_{\beta_H}^{n\downarrow}(j) p_{\beta_L}^{n\downarrow}(j') \tag{4.109}$$
$$= \sum_{j'=d^{n-m_n}+1}^{d^n} p_{\beta_L}^{n\downarrow}(j') + \sum_{i=1}^{d^{m_n}} \sum_{j=1}^{d^{n-m_n}} \left(p_{\beta_H}^{n\downarrow}(i + (j-1)d^{m_n}) - p_{\beta_H}^{n\downarrow}(j d^{m_n}) \right). \tag{4.110}$$

Since the distribution $p_{\beta_L}^{n\downarrow}$ takes the value from $j = 1$ to $j = e^{n(S(p_{\beta_L})+\epsilon)}$ except for exponentially small probability, the probability $\sum_{j=d^{n-m_n}+1}^{d^n} p_{\beta_L}^{n\downarrow}(j)$ goes to zero exponentially when $m_n < n((1 - \frac{S(\rho_{{\rm G},\beta_L})}{\log d}) - \epsilon)$.

Although the distribution $p_{\beta_H}^{n\downarrow}$ has d^n events, the probabilities $p_{\beta_H}^{n\downarrow}(k)$ take at most $(n+1)^{d-1}$ distinct values due to the combinatorics. That is, when we fix the value of i, $p_{\beta_H}^{n\downarrow}(i + d^{m_n}(j-1)) - p_{\beta_H}^{n\downarrow}(d^{m_n} j)$ takes non-zero values for at most $(n+1)^{d-1}$ elements for j. Therefore,

$$\sum_{i=1}^{d^{m_n}} \sum_{j=1}^{d^{n-m_n}} (p_{\beta_H}^{n\downarrow}(i + d^{m_n}(j-1)) - p_{\beta_H}^{n\downarrow}(d^{m_n} j)) \le d^{m_n}(n+1)^{d-1} p_{\beta_H}^{n\downarrow}(1) = d^{m_n}(n+1)^{d-1} (\max_i p_{\beta_H}(i))^n, \tag{4.111}$$

which goes to zero exponentially in the case of $m_n < -n \left(\frac{\log \max_j \{p_{\beta_H}(j)\}_{j=1}^d}{\log d} + \epsilon \right)$. Thus, when (4.104) holds, the equation (4.105) is valid. □

Now, we have complteted the preparation for the calculation of (4.38) and (4.39). Let us calculate them.

Lemma 12. *When $P_{\rm fin}^{B_H B_L}$ satisfies $P_{\rm fin}^{B_H B_L}(j_H, j_L) = \sum_{j'_H, j'_L} T_{m_n}(j_H, j_L | j'_H, j'_L) p_{{\rm G},\beta_H}^{n\downarrow}(j'_H) p_{{\rm G},\beta_L}^{n\downarrow}(j'_L)$ and the sequence $\{m_n\}$ satisfies* (4.104),

$$D(P_{\rm fin}^{B_H B_L} \| p_{{\rm G},\beta_H}^{n\downarrow} p_{{\rm G},\beta_L}^{n\downarrow}) = D_{B_H}(m_n) + D_{B_H}(m_n) + O(e^{-n\alpha_2}) \tag{4.112}$$
$$\beta_H Q_{H,n}(V_n(m_n)) = m_n \log d - D_{B_H}(m_n) + O(e^{-n\alpha_3}) \tag{4.113}$$

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

$$D_{B_H}(m_n) := \sum_{j=1}^{d^n} p_{\beta_H}^{n\downarrow}(j) \log \frac{d^{m_n} p_{\beta_H}^{n\downarrow}(j)}{p_{\beta_H}^{n\downarrow}(\lceil d^{-m_n} j \rceil)} \tag{4.114}$$
$$D_{B_L}(m_n) := \sum_{j=1}^{d^n} p_{\beta_H}^{n\downarrow}(j) \log \frac{p_{\beta_H}^{n\downarrow}(j)}{d^{m_n} p_{\beta_H}^{n\downarrow}(d^{m_n} j)}, \tag{4.115}$$

where $\lceil x \rceil$ is the ceiling function of x.

Proof: First, we define

$$\tilde{D}_{B_H}(m_n) :=:= D(\tilde{P}_{\text{fin}}^{B_H} \| p_{\text{G},\beta_H}^{n\downarrow}) \tag{4.116}$$

$$= \sum_{j=1}^{d^n} \tilde{P}_{\text{fin}}^{B_H}(j) \log \frac{\tilde{P}_{\text{fin}}^{B_H}(j)}{p_{\text{G},\beta_H}^{n\downarrow}(j)} \tag{4.117}$$

$$= \sum_{j'=1}^{d^{n-m_n}} d^{m_n} p_{\beta_H}^{n\downarrow}(d^{m_n} j') \log \frac{d^{m_n} p_{\beta_H}^{n\downarrow}(d^{m_n} j')}{p_{\beta_H}^{n\downarrow}(j')}$$

$$= \sum_{j=1}^{d^n} p_{\beta_H}^{n\downarrow}(d^{m_n} \lceil d^{-m_n} j \rceil) \log \frac{d^{m_n} p_{\beta_H}^{n\downarrow}(d^{m_n} \lceil d^{-m_n} j \rceil)}{p_{\beta_H}^{n\downarrow}(\lceil d^{-m_n} j \rceil)}. \tag{4.118}$$

Since $\sum_{j=1}^{d^{m_n}} |p_{\beta_H}^{n\downarrow}(d^{m_n} \lceil d^{-m_n} j \rceil) - p_{\beta_H}^{n\downarrow}(j)|$ is exponentially small and the difference between $\log \frac{d^{m_n} p_{\beta_H}^{n\downarrow}(d^{m_n} \lceil d^{-m_n} j \rceil)}{p_{\beta_H}^{n\downarrow}(\lceil d^{-m_n} j \rceil)}$ and $\log \frac{d^{m_n} p_{\beta_H}^{n\downarrow}(j)}{p_{\beta_H}^{n\downarrow}(\lceil d^{-m_n} j \rceil)}$ is linear with respect to n at most, the difference $\tilde{D}_{B_H}(m_n) - D_{B_H}(m_n)$ is exponentially small. Similarly, we define

$$\tilde{D}_{B_L}(m_n) := D(\tilde{P}_{\text{fin}}^{B_L} \| p_{\text{G},\beta_L}^{n\downarrow}). \tag{4.119}$$

Then, the difference $\tilde{D}_{B_L}(m_n) - D_{B_L}(m_n)$ is exponentially small. Therefore, it is sufficient for (4.114) to show that

$$D(P_{\text{fin}}^{B_H B_L} \| p_{\text{G},\beta_H}^{n\downarrow} p_{\text{G},\beta_L}^{n\downarrow}) \quad = \quad \tilde{D}_{B_H}(m_n) + \tilde{D}_{B_H}(m_n) + O(e^{-n\alpha_2}). \tag{4.120}$$

Using Lemma 11, we show (4.112) as follows. Because of Fannes's theorem [60], the equation $S(P_{\text{fin}}^{B_H B_L}) - S(\tilde{P}_{\text{P}}^{B_H} \otimes \tilde{P}_{\text{fin}}^{B_L}) = O(ne^{-n\alpha_1})$ follows from (4.105). Here, remember that the operator norm $\|Y\|$ of Y satisfies the inequality $\operatorname{tr}[XY] \le \|X\|_1 \|Y\|$. Then, the maximum $E_{\max}$ of the eigenvalues of H_B satisfies the inequality $|\sum_{j_H,j_L} [(\tilde{P}_{\text{fin}}^{B_H}(j_H) \tilde{P}_{\text{fin}}^{B_L}(j_L) - P_{\text{fin}}^{B_H B_L}(j_H, j_L)) \log P_{\text{ini}}^{B_H B_L}(j_H, j_L)]| \le 2n \|\tilde{P}_{\text{fin}}^{B_H} \tilde{P}_{\text{fin}}^{B_L} - P_{\text{fin}}^{B_H B_L}\|_1 \beta_L E_{\max}$. Thus, $D(\tilde{P}_{\text{fin}}^{B_H} \otimes \tilde{P}_{\text{fin}}^{B_L} \| p_{\text{G},\beta_H}^{n\downarrow} p_{\text{G},\beta_L}^{n\downarrow}) - D(P_{\text{fin}}^{B_H B_L} \| p_{\text{G},\beta_H}^{n\downarrow} p_{\text{G},\beta_L}^{n\downarrow}) = S(P_{\text{fin}}^{B_H B_L}) - S(\tilde{P}_{\text{fin}}^{B_H} \tilde{P}_{\text{fin}}^{B_L}) + \sum_{j_H,j_L} [(\tilde{P}_{\text{fin}}^{B_H}(j_H) \tilde{P}_{\text{fin}}^{B_L}(j_L) - P_{\text{fin}}^{B_H B_L}(j_H, j_L)) \log p_{\text{G},\beta_H}^{n\downarrow}(j_H) p_{\text{G},\beta_L}^{n\downarrow}(j_L)] = O(ne^{-n\alpha_1})$ implies (4.120), which implies (4.112).

Next, we will show (4.113). We deformate $\beta_H Q_{H,n} - m_n \log d - \tilde{D}_{B_H}(m_n)$ as follows;

$$\beta_H Q_{H,n} - m_n \log d + \tilde{D}_{B_H}(m_n) = S(P_{\text{fin}}^{B_H}) - S(\tilde{P}_{\text{fin}}^{B_H}) + \sum_{j_H,j_L} [(P_{\text{fin}}^{B_H}(j_H) - P_{\text{fin}}^{B_L}(j_L)) \log p_{\text{G},\beta_H}^{n\downarrow}(j_H)]. \tag{4.121}$$

Therefore, similar to (4.120), we find that $\beta_H Q_{H,n} - m_n \log d - \tilde{D}_{B_H}(m_n)$ is exponentially small. Since the difference $\tilde{D}_{B_H}(m_n) - D_{B_H}(m_n)$ is also exponentially small, We obtain (4.113). □

4.2.6.2 Calculation of $D_{B_H}(m_n)$ and $D_{B_L}(m_n)$

In the present subsubsection, we will prove the following lemma, which gives the concrete values of $D_{B_H}(m_n)$ and $D_{B_L}(m_n)$. In the proof of the following lemma, we will use the asymptotic expansions of $-\log p_{\text{G},\beta_H}^{n\downarrow}(j)$ and $\log j$ by using the strong large deviation theory by Bahadur and Rao [46, 47]. We will also see that the difference of the fourth constant order terms in the asymptotic expansions generates the second order term of (4.92).

Lemma 13. *When $m_n = o(n)$,*

$$D_{B_H}(m_n) =(m_n \log d)^2 n^{-1} \frac{\psi'_H(-S_H)}{2} + (m_n \log d)^3 n^{-2} (\frac{\psi''_H(-S_H)}{6} - \frac{\psi'_H(-S_H)^2}{2}) + (m_n \log d)^2 n^{-2} (\frac{\psi''_H(-S_H)}{2\psi'_H(-S_H)} - \psi'_H(-S_H))^2 + O(m_n^3 n^{-5/2}) + O(m_n^4 n^{-3}), . \tag{4.122}$$

$$D_{B_L}(m_n) =(m_n \log d)^2 n^{-1} \frac{\psi'_L(-S_L)}{2} + (m_n \log d)^3 n^{-2} (-\frac{\psi''_L(-S_L)}{6} + \frac{\psi'_L(-S_L)^2}{2}) + (m_n \log d)^2 n^{-2} (\frac{\psi''_L(-S_L)}{2\psi'_L(-S_L)} - \psi'_L(-S_L))^2 + O(m_n^3 n^{-5/2}) + O(m_n^4 n^{-3}) \tag{4.123}$$

Firstly, let us prove (4.92) by using Lemma 12 and Lemma 13.

Proof of (4.92)**:** To show (4.92), we choose

$$m_n = \left\lfloor \frac{\beta_H Q_{H,n} + \frac{\psi'_H(-S_H)}{2n} \beta_H^2 Q_{H,n}^2}{\log d} \right\rfloor . \tag{4.124}$$

Then,

$$\begin{aligned} Q_{H,n}(T_{m_n}) = Q_{H,n}(V_n(m_n)) &\overset{(a)}{=} \frac{m_n \log d}{\beta_H} - \frac{D_{B_H}(m_n)}{\beta_H} + O(e^{-n\alpha_3}) \\ &\overset{(b)}{=} \frac{m_n \log d}{\beta_H} - (m_n \log d)^2 n^{-1} \frac{\psi'_H(-S_H)}{2\beta_H} + O(\frac{m_n^3}{n^2}) \\ &\overset{(c)}{=} Q_{H,n} + \frac{\beta_H Q_{H,n}^2 \psi'_H(\beta_H)}{2n} - \frac{\beta_H Q_{H,n}^2 \psi'_H(\beta_H)}{2n} + O(\frac{Q_{H,n}^3}{n^2}) + o(1) = Q_{H,n} + O(\frac{Q_{H,n}^3}{n^2}) + o(1), \end{aligned} \tag{4.125}$$

where (a), (b), and (c) follow from (4.113), (4.122), and (4.124), respectively.

Substituting the relation (4.124) into (4.122) and (4.123), we have

$$D_{B_H}(m_n) =(\beta_H Q_{H,n})^2 n^{-1} \frac{\psi'_H(-S_H)}{2} + (\beta_H Q_{H,n})^3 n^{-2} \frac{\psi''_H(-S_H)}{6} + (m_n \log d)^2 n^{-2} (\frac{\psi''_H(-S_H)}{2\psi'_H(-S_H)} - \psi'_H(-S_H))^2 + O(Q_{H,n}^3 n^{-5/2}) + O(Q_{H,n}^4 n^{-3}), \tag{4.126}$$

$$D_{B_L}(m_n) =(\beta_H Q_{H,n})^2 n^{-1} \frac{\psi'_L(-S_L)}{2} + (\beta_H Q_{H,n})^3 n^{-2} (-\frac{\psi''_L(-S_L)}{6} + \frac{\psi'_H(-S_H)\psi'_L(-S_L)}{2} + \frac{\psi'_L(-S_L)^2}{2}) + (\beta_H Q_{H,n})^2 n^{-2} (\frac{\psi''_L(-S_L)}{2\psi'_L(-S_L)} - \psi'_L(-S_L))^2 + O(Q_{H,n}^3 n^{-5/2}) + O(Q_{H,n}^4 n^{-3}). \tag{4.127}$$

Therefore, (4.82) and (4.83) imply that

$$D_{B_H}(m_n) + D_{B_L}(m_n) =c^{(1)}_{\beta_H,\beta_L} (\beta_H Q_{H,n})^2 n^{-1} + c^{(2)}_{\beta_H,\beta_L} (\beta_H Q_{H,n})^3 n^{-2} + d^{(1)}_{\beta_H,\beta_L} (\beta_H Q_{H,n})^2 n^{-2} + O(Q_{H,n}^3 n^{-5/2}) + O(Q_{H,n}^4 n^{-3}). \tag{4.128}$$

Combining (4.57) and (4.128), we obtain the evaluation (4.92) for the efficiency $\eta^{(n)}(T_{m_n})$. □

Finally, let us prove Lemma 13.

Proof of Lemma 5: We focus on the logarithmic likelihood of $p^{n,\downarrow}_{G,\beta_X}$, which can be regarded as the the logarithmic likelihood ratio between the distribution p^n_{G,β_X} and the counting measure P_C. Now, we define the random variable $Z_X := (\log p^{n,\downarrow}_{G,\beta_X}(\hat{j}) + nS_X)/\sqrt{n}$, where $\hat{j}$ is a random variable on the natural numbers $\{j\}_{j=1}^{d^n}$ that takes the value j with the probability $p^{n\downarrow}_{\mathrm{G},\beta_H}(j)$. Then, when $j = P_C\{Z_X \geq a\}$, j is the maximum integer satisfying $\log p^{n,\downarrow}_{G,\beta_X}(j) \ge -nS_X + \sqrt{n}a$. We have the relations

$$\mathbb{E}[Z_X] = 0 \tag{4.129}$$

$$\mathbb{E}[Z_X^2] = \phi_X''(1) = \frac{1}{\psi_X'(-S_X)} \tag{4.130}$$

$$\mathbb{E}[Z_X^3] = \frac{\phi_X'''(1)}{\sqrt{n}} = -\frac{\psi_X''(-S_X)}{\psi_X'(-S_X)^3\sqrt{n}}, \tag{4.131}$$

$$\mathbb{E}[Z_X^4] = 3\phi_X''(1)^2 + \frac{\phi_X''''(1)}{n} = \frac{3}{\psi_X'(-S_X)^2} + (-\frac{\psi_X'''(-S_X)}{\psi_X'(-S_X)^3} + 3\frac{\psi_X''(-S_X)^2}{\psi_X'(-S_X)^5})\frac{1}{n}, \tag{4.132}$$

where $\mathbb{E}$ is the expectation under the distribution $p^{n,\downarrow}_{G,\beta_X}$.

Next, we focus on the Legendre transform of ϕ_X, which is written as

$$\max_s sR - \phi_X(s) = \psi_X(R)R - \phi_X(\psi_X(R)). \tag{4.133}$$

We employ the strong large deviation by Bahadur and Rao [46, 47]:

$$\begin{aligned}
&\log P_C\{\log p^{n,\downarrow}_{G,\beta_X}(\hat{j}) \ge nR\} \\
=& -n(\psi_X(R)R - \phi_X(\psi_X(R))) - \log(\sqrt{2\pi n\phi_X''(\psi_X(R))}\psi_X(R)) \\
&+ \frac{1}{n\phi''(\psi_X(R))}(-\frac{5\phi'''(\psi_X(R))^2}{24\phi''(\psi_X(R))^2} + \frac{\phi''''(\psi_X(R))}{8\phi''(\psi_X(R))} - \frac{\phi'''(\psi_X(R))}{2\psi_X(R)\phi''(\psi_X(R))} - \frac{1}{\psi_X(R)^2}) \\
&+ \sum_{k=3}^{l} f_{X,k}(R)n^{1-k} + o(\frac{1}{n^{l-1}}) \\
=& -n(\psi_X(R)R - \phi_X(\psi_X(R))) - \log\sqrt{2\pi n} - \log\psi_X(R) + \frac{1}{2}\log{\psi_X}'(R)) \\
&+ \frac{1}{n}[-\frac{1}{8}\frac{\psi'''(R)}{\psi'(R)^2} + \frac{1}{6}\frac{\psi''(R)^2}{\psi'(R)^3} + \frac{1}{2}\frac{\psi''(R)}{\psi(R)\psi'(R)} - \frac{\psi'(R)}{\psi(R)^2}] \\
&+ \sum_{k=3}^{l} f_{X,k}(R)n^{1-k} + o(\frac{1}{n^{l-1}}),
\end{aligned} \tag{4.134}$$

where $f_{X,k}(R)$ is a smooth function. In the following, for a unified treatment, the functions $-(\psi_X(R)R - \phi_X(\psi_X(R)))$, $-\log\sqrt{2\pi} - \log\psi_X(R) + \frac{1}{2}\log{\psi_X}'(R))$, and $-\frac{1}{8}\frac{\psi'''(R)}{\psi'(R)^2} + \frac{1}{6}\frac{\psi''(R)^2}{\psi'(R)^3} + \frac{1}{2}\frac{\psi''(R)}{\psi(R)\psi'(R)} - \frac{\psi'(R)}{\psi(R)^2}$ are written as $f_{X,0}(R)$, $f_{X,1}(R)$, and $f_{X,2}(R)$. So, (4.134) is simplified as $\log P_C\{\log p^{n,\downarrow}_{G,\beta_H}(\hat{j}) \ge nR\} = \sum_{k=0}^{l} f_{X,k}(R)n^{1-k} - \frac{1}{2}\log n + o(\frac{1}{n^{l-1}})$.

Thus, we have

$$\begin{aligned}
&\log F_X(Z_X) := \log P_C\{\log p^{n,\downarrow}_{G,\beta_X}(\hat{j}) \ge -nS_X + \sqrt{n}Z_X\} \\
=&\sum_{k=0}^{l}\sum_{t=0}^{2(l-k)} \frac{f^{(t)}_{X,k}(-S_X)n^{1-k-\frac{t}{2}}}{t!} Z_X^t - \frac{1}{2}\log n + o(\frac{1}{n^{l-1}}).
\end{aligned} \tag{4.135}$$

To show (4.122) and (4.123), we define $\Delta_H Z_H$ and $\Delta_L Z_L$ as

$$F_H(Z_H + \Delta_H Z_H)d^{m_n} = F_H(Z_H), \tag{4.136}$$

$$F_L(Z_L)d^{m_n} = F_L(Z_L - \Delta_L(Z_L)), \tag{4.137}$$

which are equivalent with

$$m_n \log d = \log F_H(Z_H) - \log F_H(Z_H + \Delta_H Z_H) \tag{4.138}$$

$$m_n \log d = \log F_L(Z_L - \Delta_L Z_L) - \log F_L(Z_L). \tag{4.139}$$

Hence, $\Delta_H Z_H$ and $\Delta_L Z_L$ satisfy the equations

$$m_n \log d = \sum_{i=1}^{2l} \alpha_{H,i}(Z_H) \frac{(\Delta_H Z_H)^i}{i!} + o(n^{1-l}) \tag{4.140}$$

$$m_n \log d = -\sum_{i=1}^{2l} \alpha_{L,i}(Z_L) \frac{(-\Delta_L Z_L)^i}{i!} + o(n^{1-l}), \tag{4.141}$$

where $\alpha_{X,i}(Z_X) := -\sum_{k=0}^{l-\frac{i}{2}} \sum_{j=0}^{2(l-k)-i} n^{1-k-\frac{i+j}{2}} \frac{Z_X^j}{j!} f_{X,k}^{(i+j)}(-S_X)$, where $f_{X,k}^{(i)}$ is the i-th derivative of $f_{X,k}$. Due to the definition (4.136), we have

$$\begin{aligned} D_{B_H}(m_n) =& \sum_{j=1}^{d^{m_n}} p_{G,\beta_H}^{n,\downarrow}(j)(m_n \log d) + \log p_{G,\beta_H}^{n,\downarrow}(j) - \log p_{G,\beta_H}^{n,\downarrow}(\lceil d^{-m_n} j \rceil) \\ =& \mathbb{E}[(m_n \log d) + \log p_{G,\beta_H}^{n,\downarrow}(\hat{j}) - \log p_{G,\beta_H}^{n,\downarrow}(\lceil d^{-m_n} \hat{j} \rceil)] \\ =& \mathbb{E}[(m_n \log d) + (-nS + \sqrt{n} Z_H) - (-nS_H + \sqrt{n}(Z_H + \Delta_H Z_H))] = \mathbb{E}[(m_n \log d) - \sqrt{n}\Delta_H Z_H]. \end{aligned} \tag{4.142}$$

Hence, it is needed to solve the equation (4.140) with respect to $\Delta_H Z_H$. Notice that $\alpha_{X,i}(Z_X) = O(n^{1-\frac{i}{2}})$. We apply Lemma 14 to the equation (4.140) with $x = \frac{\Delta_H Z_H}{\sqrt{n}}$, $a_i = \alpha_{X,i}(Z_X) n^{\frac{i}{2}}$, and $\epsilon = \frac{m_n \log d}{n}$. Then, we obtain

$$\frac{\Delta_H Z_H}{\sqrt{n}} = \frac{m_n \log d}{\sqrt{n}\alpha_{H,1}(Z_H)} - \frac{\alpha_{H,2}(Z_H)(m_n \log d)^2}{\sqrt{n}\alpha_{H,1}^3(Z_H)} + \frac{2\alpha_{H,2}(Z_H)^2(m_n \log d)^3}{\sqrt{n}\alpha_{H,1}^5(Z_H)} - \frac{\alpha_{H,3}(Z_H)(m_n \log d)^3}{\sqrt{n}\alpha_{H,1}^4(Z_H)} + O(m_n^4 n^{-4}). \tag{4.143}$$

That is, we obtain

$$\Delta_H Z_H = \frac{m_n \log d}{\alpha_{H,1}(Z_H)} - \frac{\alpha_{H,2}(Z_H)(m_n \log d)^2}{\alpha_{H,1}^3(Z_H)} + \frac{2\alpha_{H,2}(Z_H)^2(m_n \log d)^3}{\alpha_{H,1}^5(Z_H)} - \frac{\alpha_{H,3}(Z_H)(m_n \log d)^3}{\alpha_{H,1}^4(Z_H)} + O(m_n^4 n^{-7/2}). \tag{4.144}$$

Since $S_H = -\phi'_H(1)$, using the relations (4.82) and (4.83), we have

$$f^{(j)}_{X,0}(R) =- \psi^{(j-1)}(R) \tag{4.145}$$

$$f^{(1)}_{X,1}(R) =- \frac{\psi'(R)}{\psi(R)} + \frac{\psi''(R)}{2\psi'(R)} \tag{4.146}$$

$$f^{(2)}_{X,1}(R) =- \frac{\psi''(R)\psi(R) - \psi'(R)^2}{\psi(R)^2} + \frac{\psi'''(R)\psi'(R) - \psi''(R)^2}{2\psi'(R)^2} \tag{4.147}$$

$$f^{(3)}_{X,1}(R) =- \frac{\psi(R)^2\psi'''(R) - 3\psi(R)\psi'(R)\psi''(R) + 2\psi'(R)^3}{\psi(R)^3} + \frac{\psi'(R)^2\psi''''(R) - 3\psi'(R)\psi''(R)\psi'''(R) + 2\psi''(R)^3}{2\psi'(R)^3} \tag{4.148}$$

$$\begin{aligned} f^{(1)}_{X,2}(R) =& - \frac{1}{8}\frac{\psi'(R)\psi''''(R) - 2\psi'''(R)\psi''(R)}{\psi'(R)^3} + \frac{1}{6}\frac{2\psi'(R)\psi''(R)\psi'''(R) - 3\psi''(R)^3}{\psi'(R)^4} \\ &+ \frac{1}{2}\frac{\psi(R)\psi'(R)\psi'''(R) - \psi'(R)^2\psi''(R) - \psi(R)\psi''(R)^2}{\psi(R)^2\psi'(R)^2} - \frac{\psi(R)\psi''(R) - 2\psi'(R)^2}{\psi(R)^3}, \end{aligned} \tag{4.149}$$

we have

$$\begin{aligned} \alpha_{H,1}(Z_H) =& \sqrt{n} + \psi'_H(-S_H)Z_H + \frac{1}{\sqrt{n}}(\psi'_H(-S_H) + \frac{\psi''_H(-S_H)}{2}(Z_H^2 - \frac{1}{\psi'_H(-S)})) + \frac{1}{n}(\frac{\psi'''_H(-S_H)}{6}Z_H^3 - D_{H,1}Z_H) \\ &+ \frac{1}{n^{3/2}}(\frac{\psi''''_H(-S_H)}{24}Z_H^4 - \frac{D_{H,2}}{2}Z_H^2 - D_{H,3}) + O(n^{-2}) \end{aligned} \tag{4.150}$$

$$\alpha_{H,2}(Z_H) =\frac{\psi'_H(-S_H)}{2} + \frac{\psi''_H(-S_H)}{2\sqrt{n}}Z_H + \frac{1}{n}(\frac{\psi'''_H(-S_H)}{4}Z_H^2 - \frac{D_{H,1}}{2}) + O(n^{-3/2}) \tag{4.151}$$

$$\alpha_{H,3}(Z_H) =\frac{1}{\sqrt{n}}\frac{\psi''_H(-S)}{6} + O(n^{-1}), \tag{4.152}$$

where

$$D_{H,1} :=- \psi''_H(-S_H) + \psi'_H(-S_H)^2 + \frac{1}{2}\frac{\psi'''_H(-S_H)\psi'_H(-S_H) - \psi''_H(-S_H)^2}{\psi'_H(-S_H)^2} \tag{4.153}$$

$$\begin{aligned} D_{H,2} :=& - \psi'''(-S_H) + 3\psi'(-S_H)\psi''(-S_H) - 2\psi'(-S_H)^3 \\ &+ \frac{\psi'(-S_H)^2\psi''''(-S_H) - 3\psi'(-S_H)\psi''(-S_H)\psi'''(-S_H) + 2\psi''(-S_H)^3}{2\psi'(-S_H)^3} \end{aligned} \tag{4.154}$$

$$\begin{aligned} D_{H,3} :=& - \frac{1}{8}\frac{\psi'(-S_H)\psi''''(-S_H) - 2\psi'''(-S_H)\psi''(-S_H)}{\psi'(-S_H)^3} + \frac{1}{6}\frac{2\psi'(-S_H)\psi''(-S_H)\psi'''(-S_H) - 3\psi''(-S_H)^3}{\psi'(-S_H)^4} \\ &+ \frac{1}{2}\frac{\psi'(-S_H)\psi'''(-S_H) - \psi'(-S_H)^2\psi''(-S_H) - \psi''(-S_H)^2}{\psi'(-S_H)^2} - \psi''(-S_H) + 2\psi'(-S_H)^2. \end{aligned} \tag{4.155}$$

We have

$$\begin{aligned} \frac{m_n \log d}{\alpha_{H,1}(Z_H)} =& m_n \log d\Big[n^{-1/2} - n^{-1}\psi'_H(-S_H)Z_H + n^{-3/2}(-\frac{\psi''_H(-S_H)}{2} + \psi'_H(-S_H)^2)(Z_H^2 - \frac{1}{\psi'_H(-S_H)}) \\ &+ n^{-2}(-\frac{\psi'''_H(-S_H)}{6} - \psi'_H(-S_H)^3 + \psi''_H(-S_H)\psi'_H(-S_H))Z_H^3 \\ &+ n^{-2}(D_{H,1} + 2\psi'_H(-S_H)^2 - \psi''_H(-S_H))Z_H \\ &+ n^{-5/2}\Big((\psi'_H(-S_H)^4 - \frac{3}{2}\psi'_H(-S_H)^2\psi''_H(-S_H) + \frac{1}{4}\psi''_H(-S_H)^2 + \frac{1}{3}\psi'_H(-S_H)\psi'''_H(-S_H) - \frac{1}{24}\psi''''_H(-S_H))Z_H^4 \\ &+ (-3\psi'_H(-S_H)^3 + \frac{5}{2}\psi'_H(-S_H)\psi''_H(-S_H) - \frac{1}{2\psi'_H(-S_H)}\psi''_H(-S_H)^2 - 2\psi'_H(-S_H)D_{H,1} + \frac{D_{H,2}}{2})Z_H^2 \\ &+ (\psi'_H(-S_H) - \frac{\psi''_H(-S_H)}{2\psi'_H(-S_H)})^2 + D_{H,3}\Big)\Big] + O(m_n n^{-3}) \end{aligned}$$

and

$$
\begin{aligned}
\frac{\alpha_{H,2}(Z_H)(m_n\log d)^2}{\alpha^3_{H,1}(Z_H)} =&(m_n\log d)^2\Big[n^{-3/2}\frac{\psi'_H(-S_H)}{2}+n^{-2}(-\frac{3\psi'_H(-S_H)^2}{2}+\frac{\psi''_H(-S_H)}{2})Z_H\\
&+n^{-5/2}(\frac{\psi'''_H(-S_H)}{4}-\frac{9}{4}\psi'_H(-S_H)\psi''_H(-S_H)+3\psi'_H(-S_H)^3)Z_H^2\\
&-\frac{D_{H,1}}{2}-\frac{3}{2}\psi'_H(-S_H)^2+\frac{3}{4}\psi''_H(-S_H)\Big]+O(m_n^2n^{-3})\\
\frac{2\alpha_{H,2}(Z_H)^2(m_n\log d)^3}{\alpha^5_{H,1}(Z_H)} =&(m_n\log d)^3n^{-5/2}\frac{\psi'_H(-S_H)^2}{2}+O(m_n^3n^{-3})\\
\frac{\alpha_{H,3}(Z_H)(m_n\log d)^3}{\alpha^4_{H,1}(Z_H)} =&(m_n\log d)^3n^{-5/2}\frac{\psi''_H(-S_H)}{6}+O(m_n^3n^{-3}).
\end{aligned}
$$

Therefore,

$$
\begin{aligned}
&m_n\log d-\sqrt{n}\Delta Z_H\\
&=m_n\log d\Big[n^{-1/2}\psi'_H(-S_H)Z_H-n^{-1}(-\frac{\psi''_H(-S_H)}{2}+\psi'_H(-S_H)^2)(Z_H^2-\frac{1}{\psi'_H(-S_H)})\\
&-n^{-3/2}(-\frac{\psi'''_H(-S_H)}{6}-\psi'_H(-S_H)^3+\psi''_H(-S_H)\psi'_H(-S_H))Z_H^3\\
&-n^{-3/2}(D_{H,1}+2\psi'_H(-S_H)^2-\psi''_H(-S_H))Z_H\\
&-n^{-2}\Big((\psi'_H(-S_H)^4-\frac{3}{2}\psi'_H(-S_H)^2\psi''_H(-S_H)+\frac{1}{4}\psi''_H(-S_H)^2+\frac{1}{3}\psi'_H(-S_H)\psi'''_H(-S_H)-\frac{1}{24}\psi''''_H(-S_H))Z_H^4\\
&+(-3\psi'_H(-S_H)^3+\frac{5}{2}\psi'_H(-S_H)\psi''_H(-S_H)-\frac{1}{2\psi'_H(-S_H)}\psi''_H(-S_H)^2-2\psi'_H(-S_H)D_{H,1}+\frac{D_{H,2}}{2})Z_H^2\\
&+(\psi'_H(-S_H)-\frac{\psi''_H(-S_H)}{2\psi'_H(-S_H)})^2+D_{H,3}\Big)\Big]\\
&+(m_n\log d)^2\Big[n^{-1}\frac{\psi'_H(-S_H)}{2}+n^{-3/2}(-\frac{3\psi'_H(-S_H)^2}{2}+\frac{\psi''_H(-S_H)}{2})Z_H\\
&+n^{-2}(\frac{\psi'''_H(-S_H)}{4}-\frac{9}{4}\psi'_H(-S_H)\psi''_H(-S_H)+3\psi'_H(-S_H)^3)Z_H^2-\frac{D_{H,1}}{2}-\frac{3}{2}\psi'_H(-S_H)^2+\frac{3}{4}\psi''_H(-S_H)\Big]\\
&+(m_n\log d)^3n^{-2}(\frac{\psi''_H(-S_H)}{6}-\frac{\psi'_H(-S_H)^2}{2})+O(m_n^3n^{-5/2})+O(m_n^4n^{-4}).
\end{aligned}
$$

Now, we take the expectation of $m_n\log d-\sqrt{n}\Delta Z_H$ with use of (4.129), (4.130), (4.131), and (4.132). Then, the coefficient of the term $(m_n\log d)n^{-2}$ equals

$$
\begin{aligned}
&(-\frac{\psi'''_H(-S_H)}{6}-\psi'_H(-S_H)^3+\psi''_H(-S_H)\psi'_H(-S_H))\frac{\psi''_H(-S_H)}{\psi'_H(-S_H)^3}\\
&-3\frac{1}{\psi'_H(-S_H)^2}(\psi'_H(-S_H)^4-\frac{3}{2}\psi'_H(-S_H)^2\psi''_H(-S_H)+\frac{1}{4}\psi''_H(-S_H)^2+\frac{1}{3}\psi'_H(-S_H)\psi'''_H(-S_H)-\frac{1}{24}\psi''''_H(-S_H))\\
&-\frac{1}{\psi'_H(-S_H)}(-3\psi'_H(-S_H)^3+\frac{5}{2}\psi'_H(-S_H)\psi''_H(-S_H)-\frac{1}{2\psi'_H(-S_H)}\psi''_H(-S_H)^2-2\psi'_H(-S_H)D_{H,1}+\frac{D_{H,2}}{2})\\
&-(\psi'_H(-S_H)-\frac{\psi''_H(-S_H)}{2\psi'_H(-S_H)})^2-D_{H,3}\\
=&0.
\end{aligned}
$$

Therefore, we have

$$
\begin{aligned}
\mathbb{E}[m_n \log d - \sqrt{n}\Delta Z_H] =&(m_n \log d)^2 n^{-1} \frac{\psi'_H(-S_H)}{2} + (m_n \log d)^3 n^{-2} (\frac{\psi''_H(-S_H)}{6} - \frac{\psi'_H(-S_H)^2}{2}) \\
&+ (m_n \log d)^2 n^{-2} \Big[\frac{\psi'''_H(-S_H)}{4\psi'_H(-S_H)} - \frac{9}{4}\psi''_H(-S_H) + 3\psi'_H(-S_H)^2 - \frac{D_{H,1}}{2} - \frac{3}{2}\psi'_H(-S_H)^2 + \frac{3}{4}\psi''_H(-S_H) \Big] \\
&+ O(m_n^3 n^{-5/2}) + O(m_n^4 n^{-4}) \\
=&(m_n \log d)^2 n^{-1} \frac{\psi'_H(-S_H)}{2} + (m_n \log d)^3 n^{-2} (\frac{\psi''_H(-S_H)}{6} - \frac{\psi'_H(-S_H)^2}{2}) \\
&+ (m_n \log d)^2 n^{-2} (\frac{\psi''_H(-S_H)}{2\psi'_H(-S_H)} - \psi'_H(-S_H))^2 \\
&+ O(m_n^3 n^{-5/2}) + O(m_n^4 n^{-4}).
\end{aligned} \tag{4.156}
$$

Hence, we obtain (4.122).

Similar to (4.142), due to the definition (4.137), we have

$$
D_{B_L}(m_n) =\mathbb{E}[-(m_n \log d) + \sqrt{n}\Delta_L Z_L]. \tag{4.157}
$$

Following the same way as (4.122), we obtain (4.123) by solving (4.141).

4.2.6.2 Perturbation for higher order equation

Lemma 14. *Consider the equation*

$$
\epsilon = \sum_{i=1}^{l} a_i x^i. \tag{4.158}
$$

When ϵ is sufficiently small, the solution x is approximated as

$$
x = \sum_{i=1}^{l} \epsilon^i x_i + O(\epsilon^{l+1}). \tag{4.159}
$$

where x_1 is given as $\frac{1}{a_1}$ and x_l with $l \geq 2$ is inductively given as $-\frac{1}{a_1} \sum_{i_1,i_2,\ldots,i_{l-1}:\sum_{k=1}^{l-1} k i_k = l} a_{\sum_{k=1}^{l-1} i_k} \frac{(\sum_{k=1}^{l-1} i_k)!}{\prod_{k=1}^{l-1} i_k!} \prod_{k=1}^{l-1} x_k^{i_k}$. Specially, x_2 and x_3 are given as

$$
x_2 = -\frac{1}{a_1} x_1^2 = -\frac{1}{a_1^3} \tag{4.160}
$$

$$
x_3 = -\frac{1}{a_1}(x_1^3 + 2x_1 x_2) = -\frac{1}{a_1^4} + \frac{2}{a_1^5}. \tag{4.161}
$$

This lemma can be shown as follows. First, we substitute (4.159) into (4.158). Then, compare the coefficients with the order ϵ^i. Hence, we obtain $x_l = -\frac{1}{a_1} \sum_{i_1,i_2,\ldots,i_{l-1}:\sum_{k=1}^{l-1} k i_k = l} a_{\sum_{k=1}^{l-1} i_k} \frac{(\sum_{k=1}^{l-1} i_k)!}{\prod_{k=1}^{l-1} i_k!} \prod_{k=1}^{l-1} x_k^{i_k}$.

Chapter 5

Summary and future works

In the present thesis, we solved two theoretical problems about the quantum heat engines by using quantum information theory.

First, we have reconsidered the formulation of the work extraction from the viewpoint of quantum measurement theory, and clarified a serious conflict between the internal unitary scenario and the fully quantum scenario. We give a trade-off inequality which means that we have to destroy the coherence of the thermodynamic system in order to know the amount of the extracted energy; namely, a work extraction must be a measurement. Based on the fact, we have formularized the work extractions as a measurement process, and putted the previous formulations in order in a hierarchical structure. As a by-product, our formulation gives us a powerful tool to analyze the thermodynamic features of quantum heat engines; when the initial state is classical, we can analyze the classical model as a substitution for quantum heat engines.

Second, we have assessed how accurately thermodynamics gives an approximation to the optimal efficiency of heat engines composed of a finite-particle working body and finite-particle heat baths, by using large deviation theory. We microscopically derive a thermodynamical upper bound for the efficiency of finite-size heat engines with two heat baths that are composed of n identical particles. It is not the upper limit, but we can obtain an asymptotic approximation of the true upper limit by expanding our upper bound asymptotically in terms of $q_n := Q_{H,n}/n$, where $Q_{H,n}$ is the extracted heat from the hot bath. Thus, the difference between the thermodynamical upper bound and the true upper limit is at most in the order of $O(q_n^2)$ in case of the particles in each heat baths does not interact with each others. Our results also include another proof of the achievability of the Carnot efficiency in the macroscopic limit, and the first example of quantitative understanding of thermodynamic laws for the quantum systems which consist of many, but finite praticles.

Finally, as the discussion, we introduce two future works.

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.

Reconstruction of the information thermodynamics

Because every work extraction is a measurement process in our formulation, the information thermodynamics should be reconstructed in our formulation. Note that the information which is obtained by the measurement process can be used in two ways; one is used to know Therefore, there might be a trade-off relation between how much we can extract work and how precice we can know the amount of the extracted work.

Appendix A

The comparison (2.16) with (2.65) in terms of achievability

In the present appendix, we prove that the converse of the corollary 1 is not true. To be concrete, we prove the following two theorems;

Theorem 8. *When the following conditions are satisfied, we can always achieve the equality of Eq.* (2.65) *with proper choices of* $\{\hat{P}_{(k)}\}$ *and* $\{\hat{U}_{(k)}\}$ *for any* $\hat{U}_{SM}$*:*

Condition 1*: The system S is a two-level system.*

Condition 2*: We omit Step 1 in the isothermal operation with feedback control which is defined in the subsection 2.2.1. Namely, we use* $\rho_{\rm i}$ *as* ρ_1*.*

Condition 3*: During the measurement* $\{\mathcal{E}_j\}$ *in Step 2, the system S and the heat bath B does not interact with each others.*

Condition 3 implies that the system and baths do not interact during the measurement; if the system and baths interact during the measurement, the information obtained by the memory contains the information about the system as well as about the baths.

Theorem 9. *Under Conditions 1–3, there is a measurement* $\{\mathcal{E}_{(j)}\}$ *for which we cannot achieve the equality of Eq.* (2.16) *with any* $\hat{U}_{(j)}$*.*

We prove Theorem 8 by using the following lemma;

Lemma 15. *For an arbitrary three-qubit pure state* $|\psi_{MSR_1}\rangle$*, there exists a projective measurement* $\{\tilde{P}_{(k)}\}_{k=0,1}$ *such that the results* $\frac{\tilde{P}_{(k)}}{\sqrt{p_k}}|\psi_{MSR_1}\rangle$ *are LU-equivalent for* $k=0,1$ *and*

$$E^{S\text{-}R_1}(\frac{\tilde{P}_{(k)}}{\sqrt{p_k}}|\psi_{MSR_1}\rangle) = E_F^{S\text{-}R_1}(\hat{\rho}_{SR_1}) \tag{A.1}$$

is valid, where $\hat{\rho}_{SR_1} := {\rm tr}_M[|\psi_{MSR_1}\rangle\langle\psi_{MSR_1}|]$*.*

Proof of Theorem 8: In order to perform the proof, we firstly introduce the reference systems R_1 and R_2, and the pure states $|\psi_{SR_1}\rangle$ and $|\psi_{BR_1}\rangle$ of SR_1 and SR_2 such that

$${\rm tr}_{R_1}[|\psi_{SR_1}\rangle\langle\psi_{SR_1}|] = \frac{\exp(-\beta H_1^S)}{Z^S(H_{\rm i}^S,\beta)}, \quad {\rm tr}_{R_2}[|\psi_{BR_2}\rangle\langle\psi_{BR_2}|] = \frac{\exp(-\beta H_1^B)}{Z^B(H^B,\beta)} \tag{A.2}$$

Because of Condition 2, the premeasurement state of $MSBR_1R_2$ is $|0_M\rangle \otimes |\psi_{SR_1}\rangle \otimes |\psi_{BR_1}\rangle$. Because of Condition 3, after the unitary interaction U_{SM}, the state of $MSBR_1R_2$ becomes $U_{SM}(|0_M\rangle \otimes |\psi_{SR_1}\rangle) \otimes |\psi_{BR_1}\rangle$. Thus, the following equality holds;

$$-\Delta E_F^{SB-R} = -\Delta E_F^{S-R}. \tag{A.3}$$

Let us take the projective measurement $\{\tilde{P}_{(k)}\}$ for $|\psi'_{MSR_1}\rangle := U_{SM}(|0_M\rangle \otimes |\psi_{SR_1}\rangle)$, and perform it on the memory M. Because the system S is a qubit, and because $\frac{\tilde{P}_{(k)}}{\sqrt{p_k}}|\psi'_{MSR_1}\rangle$ are LU-equivalent for $k = 0, 1$, there exist the unitary transformations $V_{(k)}$ on S such that

$$\frac{1}{p_0}\mathrm{tr}_{R_1}[V_{(0)}\tilde{P}_{(0)}|\psi'_{MSR_1}\rangle\langle\psi'_{MSR_1}|\tilde{P}_{(0)}V_{(0)}^{\dagger}] = \frac{1}{p_1}\mathrm{tr}_{R_1}[V_{(1)}\tilde{P}_{(1)}|\psi'_{MSR_1}\rangle\langle\psi'_{MSR_1}|\tilde{P}_{(1)}V_{(1)}^{\dagger}] = \rho_{\mathrm{G},\beta'}(H_{\mathrm{i}}^S), \tag{A.4}$$

for an inverse temperature β' which is not always equal to β. Because S is a qubit, we can turn $\rho_{\mathrm{G},\beta'}(H_{\mathrm{i}}^S)$ into $\rho_{\mathrm{G},\beta'}(H_{\mathrm{f}}^S)$ by adiabatic transformation V on S, with a proper Hamiltonian H_{f}^S.

Let us show that the projective measurement $\{\tilde{P}_{(k)}\}$ and the feedback $\{VV_{(k)}\}$ satisfy the equality of (2.65). Because of (A.1), the $\{\tilde{P}_{(k)}\}$ is the projective measurement which achieves the equality of (2.58). Moreover, because the state of S becomes the Gibbs state whose inverse temperature β after the feedback $VV_{(k)}$, the sum $\sum_j p_j D(\rho_{\mathrm{f}}^j \| \rho_{\mathrm{G},\beta}(H_{\mathrm{f}}^S))$ is equal to zero. Thus, (2.24) yields

$$W_{\mathrm{fb}} = -\frac{1}{\beta}\Delta E_F^{SB-R} - \Delta F^S(\beta). \tag{A.5}$$

Thus, $\{\tilde{P}_{(k)}\}$ and $\{\hat{V}_{(k)}\}$ are the measurement and feedback that we want.□

Proof of Theorem 9: It is sufficient to prove the existence of a counterexample of the measurement $\{\mathcal{E}_{(j)}\}$. Because of (2.24), the equality of Eq. (2.16) is valid only if there exists a set of unitary transformations $\{\hat{U}_{(k)}\}$ that satisfy

$$\sum_j p_j D(\rho_{\mathrm{f}}^j \| \rho_{\mathrm{G},\beta}(H_{\mathrm{f}}^S)) = 0. \tag{A.6}$$

Because $D(\hat{\rho}||\hat{\rho}') = 0$ if and only if $\hat{\rho} = \hat{\rho}'$, the equality (A.6) means that every ρ_2^j are LU-equivalent for $j = 0, 1$, in other words, the measurement $\{\mathcal{E}_{(j)}\}$ is a deterministic measurement. Because of this logic, if Theorem 9 were not valid, any measurement $\{\mathcal{E}_{(j)}\}$ would be deterministic. This is clearly false, and thus Theorem 9 holds.□

Proof of Lemma 15: Because $\hat{\rho}_{SR_1}$ is a two-qubit mixed state, we can express $E_F^{S\text{-}R_1}(\hat{\rho}_{SR_1})$ in the form of the concurrence [55]:

$$E_F^{S\text{-}R_1}(\hat{\rho}_{SR_1}) = h\left(\frac{1 + \sqrt{1 - C_{SR_1}^2(\hat{\rho}_{SR_1})}}{2}\right), \tag{A.7}$$

where $C_{SR_1}(\hat{\rho}_{SR_1})$ is the concurrence of $\hat{\rho}_{SR_1}$ and $h(x) \equiv -x\log x - (1-x)\log(1-x)$. Thus, we only have to find a projective measurement $\{\tilde{P}_{(k)}\}_{k=0,1}$ such that $\tilde{P}_{(k)}|\psi_{MSR_1}\rangle$ for $k = 0, 1$ are LU-equivalent to each other and $C_{SR_1}(\tilde{P}_{(k)}|\psi_{MSR_1}\rangle) = C_{SR_1}(\hat{\rho}_{SR_1})$.

Before giving the projective measurement $\{\tilde{P}_{(k)}\}$, we first present preparations. First we express $|\psi_{MSR_1}\rangle$ in the form of the generalized Schmidt decomposition [64]:

$$\begin{aligned}|\psi_{MSR_1}\rangle &= \lambda_0|000\rangle + \lambda_1 e^{i\varphi}|100\rangle + \lambda_2|101\rangle \\ &\quad + \lambda_3|110\rangle + \lambda_4|111\rangle \quad (0 \le \varphi \le \pi)\end{aligned} \tag{A.8}$$

and introduce the following eight parameters [62];

$$
\begin{aligned}
K_{MS} &\equiv C_{MS}^2 + \tau_{MSR_1}, && \text{(A.9)}\\
K_{MR_1} &\equiv C_{MR_1}^2 + \tau_{MSR_1}, && \text{(A.10)}\\
K_{SR_1} &\equiv C_{SR_1}^2 + \tau_{MSR_1}, && \text{(A.11)}\\
J_5 &\equiv 4\lambda_0^2(|\lambda_1\lambda_4 e^{i\varphi} - \lambda_2\lambda_3|^2 + \lambda_2^2\lambda_3^2 - \lambda_1^2\lambda_4^2), && \text{(A.12)}\\
K_5 &\equiv J_5 + \tau_{MSR_1}, && \text{(A.13)}\\
\Delta_J &\equiv K_5^2 - K_{MS}K_{MR_1}K_{SR_1}, && \text{(A.14)}\\
e^{-i\tilde{\varphi}_5} &\equiv \frac{\lambda_2\lambda_3 - \lambda_1\lambda_4 e^{i\varphi}}{|\lambda_2\lambda_3 - \lambda_1\lambda_4 e^{i\varphi}|}, && \text{(A.15)}\\
Q_{\mathrm{e}} &\equiv \mathrm{sgn}\left[\sin\varphi\left(\lambda_0^2 - \frac{\tau_{MSR_1} + J_5}{2(C_{SR_1}^2 + \tau_{MSR_1})}\right)\right], && \text{(A.16)}
\end{aligned}
$$

where τ_{MSR_1} is the tangle of $|\psi_{MSR_1}\rangle$ and $\mathrm{sgn}[x]$ is the sign function,

$$
\mathrm{sgn}[x] = \left\{ \begin{array}{ll} x/|x| & (x \neq 0) \\ 0 & (x = 0) \end{array} \right\}. \tag{A.17}
$$

When $Q_{\mathrm{e}} = 0$, there are two possible decompositions which satisfy Eq. (B.1). We then choose the decomposition with a greater coefficient λ_0.

Now we have completed the preparation. In the basis of Eq. (B.1), the projective measurement $\{\tilde{P}_{(k)}\}_{k=0,1}$ is given as follows:

$$
\tilde{P}_{(0)} = \sqrt{\begin{pmatrix} a & ke^{-i\theta} \\ ke^{i\theta} & b \end{pmatrix}}, \tilde{P}_{(1)} = \sqrt{\begin{pmatrix} 1-a & -ke^{-i\theta} \\ -ke^{i\theta} & 1-b \end{pmatrix}}, \tag{A.18}
$$

where the measurement parameters a, b, k and θ are defined as follows:

$$
\begin{aligned}
a &= \frac{1}{2} - \frac{K_5\tau_{MSR_1} \dot{\pm} \sqrt{\Delta_J} C_{SR_1}^2}{2K_{SR_1}\sqrt{K_5^2 - K_{MS}K_{MR_1}C_{SR_1}^2}}, && \text{(A.19)}\\
b &= 1 - a, && \text{(A.20)}\\
k &= \sqrt{a(1-a)}, && \text{(A.21)}\\
\theta &= -\tilde{\varphi}_5, && \text{(A.22)}
\end{aligned}
$$

and when $Q_{\mathrm{e}} \neq 0$ the mark $\dot{\pm}$ means $-Q_{\mathrm{e}}$ and when $Q_{\mathrm{e}} = 0$ the mark $\dot{\pm}$ means $-$. By using Eqs. (B.84)–(B.87) and Lemma 16 in Appendix B and after straightforward algebra, we can confirm that the measurement $\{\tilde{P}_{(k)}\}$ is the measurement that we sought.

Appendix B

Deterministic LOCC transformation of three-qubit pure states

In the present appendix, we give an explicit necessary and sufficient condition to determine whether a deterministic LOCC transformation from an arbitrary three-qubit pure state $|\psi\rangle$ to another arbitrary state $|\psi'\rangle$ is executable or not. The contents in the present appendix are in the sections 2, 3 and 4 of the author's result Ref. [62]

B.1 Theorems and their physical meanings

In this section, we list up Theorems in this article and describe their physical meaning.

We consider only three-qubit pure states throughout the present paper. Before listing up Theorems, we introduce a useful expression of three-qubit pure states. An arbitrary pure state $|\psi\rangle$ of the three qubits A, B and C is expressed in the form of the generalized Schmidt decomposition

$$|\psi\rangle = \lambda_0 |000\rangle + \lambda_1 e^{i\varphi} |100\rangle + \lambda_2 |101\rangle + \lambda_3 |110\rangle + \lambda_4 |111\rangle \tag{B.1}$$

with a proper basis set [64]. (There are two kinds of decompositions which are called generalization of the Schmidt decomposition. One was given in Ref. [64] and the other was given in Ref. [65]. We use the former in the present paper.) The coefficients $\{\lambda_i | i = 0, ..., 4\}$ in (B.1) are nonnegative real numbers and satisfy that $\sum_{i=0}^{4} \lambda_i^2 = 1$. Note that the phase φ can take any real values if one of the coefficients $\{\lambda_i | i = 0, ..., 4\}$ is zero, in which case we define the phase φ to be zero in order to remove the ambiguity.

Two different decompositions of the form (B.1) are possible for the same state $|\psi\rangle$, one with $0 \le \varphi \le \pi$ and the other with $\pi \le \varphi \le 2\pi$. These two decompositions are LU-equivalent; in other words, they can be transformed into each other by local unitary (LU) transformations. Hereafter, we refer to the decomposition (B.1) with $0 \le \varphi \le \pi$ as the positive decomposition and the one (B.1) with $\pi < \varphi < 2\pi$ as the negative decomposition. We also refer to the coefficients of the positive and negative decompositions as the positive-decomposition coefficients and the negative-decomposition coefficients, respectively. Therefore, a set of coefficients gives a unique set of states that are LU-equivalent to each other, whereas such a set of states may give two possible sets of coefficients: for $\varphi \ne 0$, a set of positive-decomposition coefficients and a set of negative-decomposition

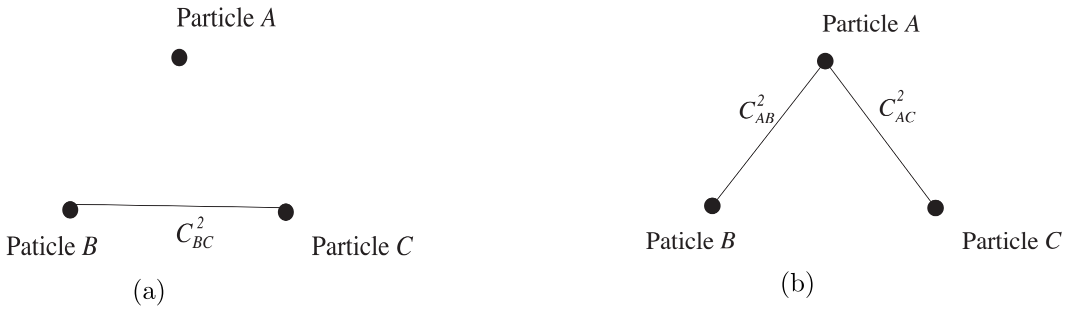

Figure B.1: The concept of (a) a biseparable state. There is no such state as (b).

coefficients are possible, while for $\varphi = 0$, two sets of positive-decomposition coefficients are possible. When $\sin\varphi \neq 0$ holds, a set of LU-equivalent states and a set of positive-decomposition coefficients have a one-to-one correspondence.

We can express the entanglement parameters in the coefficients of the generalized Schmidt decomposition:

$$C_{AB} = 2\lambda_0\lambda_3,\ \ C_{AC} = 2\lambda_0\lambda_2,\ \ C_{BC} = 2|\lambda_1\lambda_4 e^{i\varphi} - \lambda_2\lambda_3|, \tag{B.2}$$

$$\tau_{ABC} = 4\lambda_0^2\lambda_4^2, \tag{B.3}$$

$$J_5 = 4\lambda_0^2(|\lambda_1\lambda_4 e^{i\varphi} - \lambda_2\lambda_3|^2 + \lambda_2^2\lambda_3^2 - \lambda_1^2\lambda_4^2), \tag{B.4}$$

where τ is the tangle [56], C_{AB}, C_{AC} and C_{AC} are the concurrences [71], and J_5 is four times of J_5 in Ref. [64].

Finally, we define the names of types of states. We refer to a state whose τ_{ABC} is nonzero or whose C_{AB}, C_{AC} and C_{BC} are all nonzero as a truly tripartite state. We refer to a state which has only a single kind of the bipartite entanglement as a biseparable state (Fig. B.1(a)). Note that there is no state which has only two kinds of the bipartite entanglement (Fig. B.1(b)). If there were such a state as in Fig. B.1(b), the coefficients $\{\lambda_i, \varphi | i = 0, ..., 4\}$ of the state would satisfy

$$\lambda_0\lambda_2 \neq 0,\ \ \lambda_0\lambda_3 \neq 0,\ \ \lambda_0\lambda_4 = 0,\ \ |\lambda_1\lambda_4 e^{i\varphi} - \lambda_2\lambda_3| = 0, \tag{B.5}$$

but (B.5) is impossible.

The preparation has been now completed. Let us give Theorems and see their meaning.

Theorem 10. *(Condition for the LU-equivalence)*

Arbitrary three-qubit pure states are LU-equivalent if and only if their entanglement parameters $(C_{AB}, C_{AC}, C_{BC}, \tau_{ABC}, J_5,$ *are equal to each other. Here* Q_e *is a new parameter which is given by*

$$Q_e = sgn\left[\sin\varphi\left(\lambda_0^2 - \frac{\tau_{ABC} + J_5}{2(C_{BC}^2 + \tau_{ABC})}\right)\right], \tag{B.6}$$

where $sgn[x]$ *is the sign function,*

$$sgn[x] = \left\{ \begin{array}{ll} x/|x| & (x \neq 0) \\ 0 & (x = 0) \end{array} \right\}, \tag{B.7}$$

and the parameters φ *and* λ_0 *are the coefficients of the generalized Schmidt decomposition.*

Physical meaning of Theorem 10: Theorem 10 gives a necessary and sufficient condition for the LU-equivalence of three-qubit pure states. The necessary and sufficient conditions can be given in other ways. However, the parameters used in Theorem 10 have very clear physical meaning of the magnitude, phase and charge of the entanglement, in the space of the LU-equivalence class of three-qubit pure states.

The concurrences C_{AB}, C_{AC} and C_{BC} express the amount of the entanglement between the qubits A and B, A and C and B and C, respectively. The tangle τ_{ABC} expresses the amount of the entanglement among three qubits.

What about J_5? The parameter J_5 and the concurrences let us derive a phase of the entanglement as follows:

$$\cos\varphi_5 = \frac{J_5}{C_{AB}C_{AC}C_{BC}}, \ \ 0 \leq \varphi_5 \leq \pi. \tag{B.8}$$

Let us refer to the phase φ_5 as the entanglement phase (EP). The entanglement phase φ_5 is invariant with respect to local unitary operations, because all of the parameters J_5 and C_{AB} C_{AC} C_{BC} are. When $C_{AB}C_{AC}C_{BC} = 0$, the phase becomes indefinite. Hereafter, we refer to a state whose entanglement phase φ_5 is definite as an EP-definite state and to a state whose entanglement phase φ_5 is indefinite as an EP-indefinite state. An EP-indefinite state with $\tau_{ABC} \neq 0$ and an EP-definite state are truly tripartite states. A truly tripartite state is an EP-indefinite state with $\tau_{ABC} \neq 0$ or an EP-definite state. A biseparable state is EP indefinite with $\tau_{ABC} = 0$. An EP-indefinite state with $\tau_{ABC} = 0$ is a biseparable state.

Finally, we interpret the new parameter $Q_{\rm e}$. As we will prove in section B.2, the parameter $Q_{\rm e}$ is equal for the possible sets of coefficients of a state. Therefore, the parameter $Q_{\rm e}$ is invariant with respect to local unitary transformations. The parameter $Q_{\rm e}$ is a tripartite parameter, because $Q_{\rm e}$ is invariant with respect to the permutation of the qubits A, B and C. This fact is shown in Appendix A. The complex-conjugate transformation of a state does not change the parameters $(C_{AB}, C_{AC}, C_{BC}, \tau_{ABC}, J_5)$ nor λ_0, but reverses the sign of $\sin\varphi$. Thus, the complex-conjugate transformation reverses the sign of $Q_{\rm e}$. As we have seen, the parameter $Q_{\rm e}$ has characters that the electric charge has; hence, we refer to $Q_{\rm e}$ as the entanglement charge.

The next Theorem 11 gives a necessary and sufficient condition for the possibility of a deterministic LOCC. In order to express Theorem 11 in simpler forms, we define three nonnegative real-valued parameters K_{AB}, K_{AC} and K_{BC} as follows:

$$K_{AB} = C_{AB}^2 + \tau_{ABC}, \ \ K_{AC} = C_{AC}^2 + \tau_{ABC}, \ \ K_{BC} = C_{BC}^2 + \tau_{ABC}. \tag{B.9}$$

Then, the five parameters K_{AB}, K_{AC}, K_{BC}, τ_{ABC} and J_5 are independent of each other and are invariant with respect to local unitary operations. We can substitute these five parameters for the entanglement parameters $(C_{AB}, C_{AC}, C_{BC}, \tau_{ABC}, J_5)$. Let us refer to the old parameters $(C_{AB}, C_{AC}, C_{BC}, \tau_{ABC}, J_5)$ as the C-parameters and to the new parameters $(K_{AB}, K_{AC}, K_{BC}, \tau_{ABC}, J_5)$ as the K-parameters. Note that $(C_{AB}, C_{AC}, C_{BC}, \tau_{ABC}, J_5)$ and $(K_{AB}, K_{AC}, K_{BC}, \tau_{ABC}, J_5)$ have a one-to-one correspondence.

We also define three parameters in order to simplify expressions which often appear in the present paper:

$$J_{\rm ap} \equiv C_{AB}^2 C_{AC}^2 C_{BC}^2, \ \ K_{\rm ap} \equiv K_{AB}K_{AC}K_{BC}, \ \ K_5 \equiv \tau_{ABC} + J_5, \tag{B.10}$$

$$\Delta_J \equiv K_5^2 - K_{\rm ap} \geq 0, \tag{B.11}$$

where the subscript ap is abbreviation of all pairs, and where Δ_J is sixteen times of Δ_J in Ref. [64]. Note that these parameters J_{ap}, K_{ap}, K_5 and Δ_J are *not* included in the K-parameters; we introduce them only for simplicity. By definition, J_{ap}, K_{ap}, K_5 and Δ_J are invariant with respect to local unitary transformations as well as permutations of A, B and C.

Theorem 11. *(deterministic LOCC)*

A deterministic LOCC transformation from an arbitrary state $|\psi\rangle$ to another arbitrary state $|\psi'\rangle$ is executable if and only if the K-parameters of $|\psi\rangle$ and $|\psi'\rangle$ satisfy the following conditions:

Condition 1: There are real numbers $0 \le \zeta_A \le 1$, $0 \le \zeta_B \le 1$, $0 \le \zeta_C \le 1$ and $\zeta_{lower} \le \zeta \le 1$ which satisfy the following equation:

$$\begin{pmatrix} K'_{AB} \\ K'_{AC} \\ K'_{BC} \\ \tau'_{ABC} \\ J'_5 \end{pmatrix} = \zeta \begin{pmatrix} \zeta_A\zeta_B & & & & \\ & \zeta_A\zeta_C & & & \\ & & \zeta_B\zeta_C & & \\ & & & \zeta_A\zeta_B\zeta_C & \\ & & & & \zeta_A\zeta_B\zeta_C \end{pmatrix} \begin{pmatrix} K_{AB} \\ K_{AC} \\ K_{BC} \\ \tau_{ABC} \\ J_5 \end{pmatrix}, \tag{B.12}$$

where

$$\zeta_{lower} = \frac{J_{ap}}{(K_{AB} - \zeta_C\tau_{ABC})(K_{AC} - \zeta_B\tau_{ABC})(K_{BC} - \zeta_A\tau_{ABC})}. \tag{B.13}$$

Condition 2: If the state $|\psi'\rangle$ is EP definite, we check whether

$$(\Delta_J = 0) \wedge (J_{ap} - J_5^2 = 0) \tag{B.14}$$

holds or not. When (B.14) *does not hold, the condition is*

$$Q_e = Q'_e \ \textit{and} \ \zeta = \tilde{\zeta}, \tag{B.15}$$

where

$$\tilde{\zeta} \equiv \frac{K_{ap}(J_{ap} - J_5^2) + \Delta_J J_{ap}}{K_{ap}(J_{ap} - J_5^2) + \Delta_J(K_{AB} - \zeta_C\tau_{ABC})(K_{AC} - \zeta_B\tau_{ABC})(K_{BC} - \zeta_C\tau_{ABC})}. \tag{B.16}$$

When (B.14) *holds, the condition is*

$$|Q'_e| = sgn[(1-\zeta)(\zeta - \zeta_{lower})], \tag{B.17}$$

or in other expressions,

$$Q'_e \begin{cases} = 0 & (\zeta = 1 \ \textit{or} \ \zeta = \zeta_{lower}), \\ \neq 0 & (\textit{otherwise}). \end{cases} \tag{B.18}$$

Physical meaning of Theorem 11: Theorem 11 gives a necessary and sufficient condition for the possibility of a deterministic LOCC (d-LOCC) transformation. Note that the conditions are given as the condition for a diagonal matrix which relates two vectors of the K-parameters. This shows that there exists a vector structure in three-qubit pure states.

The difficulty of seeking necessary and sufficient conditions for the possibility of multipartite d-LOCC transformation lies in the fact that we cannot apply the majorization theory, which played an important part in clarifying bipartite-pure d-LOCC transformation, to multipartite pure states. The majorization theory was applied to a vector structure which exists in the coefficients of the Schmidt decomposition. Unfortunately, there is not a vector structure in the coefficients of the generalized Schmidt decomposition, but a tensor structure. Thus, the majorization theory is not applicable to three-qubit pure states directly; this was the reason of the difficulty of clarification of three-qubit d-LOCC transformation.

However, Theorem 11 implies that there is a vector structure in three-qubit states in view of the entanglement measures. Note that there is a possibility that other multipartite systems have similar structures; it is plausible that the nonlocal features of N-qubit pure states can be expressed completely in the magnitudes, phases and charges of the entanglement. Then, the approach of the present paper may be applicable to such systems.

There are two important interpretations of Theorem 11. One is the rule of the flow of the entanglement and the other is the preservation of the charge. Let us see the rule of the flow of the entanglement. Consider a d-LOCC transformation whose measurement is performed only on the qubit A. In such a case, the condition 1 reduces to the following condition $1'$: there are real numbers $0 \leq \zeta_A \leq 1$ and $\zeta_{\text{lower}} \leq \zeta \leq 1$ which satisfy the following equation:

$$\begin{pmatrix} K'_{AB} \\ K'_{AC} \\ K'_{BC} \\ \tau'_{ABC} \\ J'_5 \end{pmatrix} = \zeta \begin{pmatrix} \zeta_A & & & & \\ & \zeta_A & & & \\ & & 1 & & \\ & & & \zeta_A & \\ & & & & \zeta_A \end{pmatrix} \begin{pmatrix} K_{AB} \\ K_{AC} \\ K_{BC} \\ \tau_{ABC} \\ J_5 \end{pmatrix}, \tag{B.19}$$

where

$$\zeta_{\text{lower}} = \frac{C_{BC}^2}{(K_{BC} - \zeta_A \tau_{ABC})}. \tag{B.20}$$

Substituting the C-parameters $(C_{AB}, C_{AC}, C_{BC}, \tau_{ABC}, J_5)$ for the K-parameters in (B.19), we obtain the following condition $1''$: $0 \leq \alpha_A \leq 1$, $0 \leq \beta_A \leq 1$ which satisfy the following equation:

$$\begin{pmatrix} C'^2_{AB} \\ C'^2_{AC} \\ C'^2_{BC} \\ \tau'_{ABC} \\ J'_5 \end{pmatrix} = \begin{pmatrix} \alpha_A^2 & & & & \\ & \alpha_A^2 & & & \\ & & 1 & \beta_A(1-\alpha_A^2) & \\ & & & \alpha_A^2 & \\ & & & & \alpha_A^2 \end{pmatrix} \begin{pmatrix} C^2_{AB} \\ C^2_{AC} \\ C^2_{BC} \\ \tau_{ABC} \\ J_5 \end{pmatrix}. \tag{B.21}$$

We can interpret the above as the rule how a deterministic measurement, which is a measurement whose results can be transformed into a unique state by local unitary operations without exception, changes the entanglement. We can express this change as in Fig. B.2. After performing a deterministic measurement on the qubit A, the four entanglement parameters, C_{AB}^2, C_{AC}^2, τ_{ABC} and J_5, the last of which does not appear in Fig. B.2, are multiplied by α_A^2. Note that these four entanglement parameters are related to the qubit A, which is the measured qubit. The quantity $\beta_A(1-\alpha_A^2)\tau_{ABC}$, which is a part of the entanglement lost from τ_{ABC}, is added to C_{BC}^2, which is the only entanglement parameter that is not related to the measured qubit A. The quantity $(1-\beta_A)(1-\alpha_A^2)\tau_{ABC}$, which is the rest of the entanglement lost from τ_{ABC} disappear. We call this phenomenon the entanglement transfer.

Finally, let us see the behavior of Q_{e} when we perform a d-LOCC transformation. Hereafter, we refer to a state which satisfies (B.14) as $\tilde{\zeta}$-indefinite and refer to a state which does not satisfy (B.14) as $\tilde{\zeta}$-definite. The

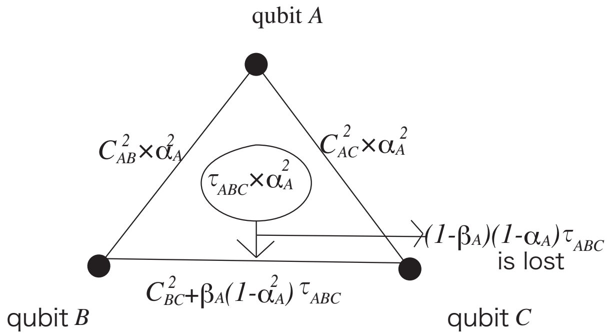

Figure B.2: Entanglement transfer

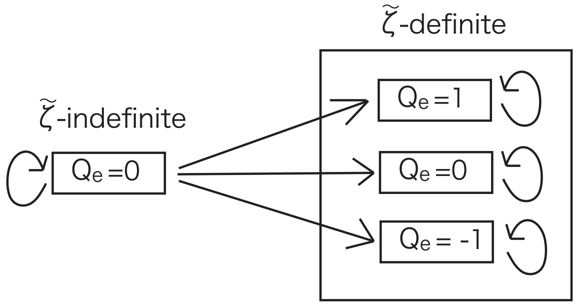

Figure B.3: The entanglement charge Q_e for $\tilde{\zeta}$-definite states and $\tilde{\zeta}$-definite states. The arrows indicate the executable deterministic LOCC transformations among truly multipartite states; transformations not in this figure are not executable as deterministic LOCC transformations. For example, we cannot transform a $\tilde{\zeta}$-definite state whose Q_e is 1 into another $\tilde{\zeta}$-definite state whose Q_e is 0.

following statements hold:

Statement $\tilde{\zeta}$-1: Any biseparable state is also a $\tilde{\zeta}$-indefinite state.

Statement $\tilde{\zeta}$-2: Any $\tilde{\zeta}$-indefinite state satisfies $Q_\mathrm{e} = 0$.

Statement $\tilde{\zeta}$-3: A d-LOCC transformation from an EP-indefinite state to an EP-definite state is executable if and only if the initial state is $\tilde{\zeta}$-indefinite.

Statement $\tilde{\zeta}$-4: Among truly multipartite states, a d-LOCC transformation from a $\tilde{\zeta}$-indefinite state to a $\tilde{\zeta}$-definite state is executable, but the contrary is not executable.

Statement $\tilde{\zeta}$-5: When the initial state is $\tilde{\zeta}$-definite, the d-LOCC transformation conserves the entanglement charge Q_e.

Because of the above five statements, the $\tilde{\zeta}$-definite state can be considered as a "charge-definite state." When we transform a $\tilde{\zeta}$-indefinite state into a $\tilde{\zeta}$-definite state, we can choose the value of the entanglement charge Q_e; once the value is determined, we cannot change it anymore with a deterministic LOCC transformation (Fig. B.3).

The third theorem gives the minimum number of times of measurements to reproduce an arbitrary deterministic LOCC transformation between three-qubit pure states.

Table B.1: The minimum number of times of measurements to reproduce an arbitrary deterministic LOCC transformation.

Initial state	Final state	Times
Truly tripartite state	Truly tripartite state	3
Truly tripartite state	Biseparable state or full-separable state	2
Biseparable state	Biseparable state or full-separable state	1
Full-separable state	Full-separable state	0

Theorem 12. *the minimum number of necessary times of measurements The minimum number of necessary times of measurements to reproduce an arbitrary deterministic LOCC transformation from an arbitrary three-qubit state $|\psi\rangle$ to another arbitrary state $|\psi'\rangle$ is given as listed in Table 1. The order of measurements are commutable; we can choose which qubit is measured first, second and third.*

B.2 Proof of Theorem 10

In this section, we prove Theorem 10. We perform the proof in the following two steps. First, we see that the C-paramters $(C_{AB}, C_{AC}, C_{BC}, \tau_{ABC}, J_5)$ does not specify an LU-equivalence class uniquely. Second, we show that the entanglement charge Q_e eliminate the non-uniqueness.

When we specify the set $(C_{AB}, C_{AC}, C_{BC}, \tau_{ABC}, J_5)$, there are still two possible positive decompositions [66]:

$$(\lambda_0^\pm)^2 = \frac{J_5 + \tau_{ABC} \pm \sqrt{\Delta_J}}{2(C_{BC}^2 + \tau_{ABC})} = \frac{K_5 \pm \sqrt{\Delta_J}}{2K_{BC}}, \tag{B.22}$$

$$(\lambda_2^\pm)^2 = \frac{C_{AC}^2}{4(\lambda_0^\pm)^2},\ (\lambda_3^\pm)^2 = \frac{C_{AB}^2}{4(\lambda_0^\pm)^2},\ (\lambda_4^\pm)^2 = \frac{\tau_{ABC}}{4(\lambda_0^\pm)^2}, \tag{B.23}$$

$$(\lambda_1^\pm)^2 = 1 - (\lambda_0^\pm)^2 - \frac{C_{AB}^2 + C_{AC}^2 + \tau_{ABC}}{4(\lambda_0^\pm)^2}, \tag{B.24}$$

$$\cos\varphi^\pm = \frac{(\lambda_1^\pm)^2(\lambda_4^\pm)^2 + (\lambda_2^\pm)^2(\lambda_3^\pm)^2 - C_{BC}^2/4}{2\lambda_1^\pm\lambda_2^\pm\lambda_3^\pm\lambda_4^\pm}, \tag{B.25}$$

where

$$0 \le \varphi^\pm \le \pi. \tag{B.26}$$

Thus, there are four possible sets of coefficients for one set of $(C_{AB}, C_{AC}, C_{BC}, \tau_{ABC}, J_5)$: the positive-decomposition coefficients $\{\lambda_i^+, \varphi^+ | i = 0, ..., 4\}$ and $\{\lambda_i^-, \varphi^- | i = 0, ..., 4\}$ as well as other two sets of coefficients $\{\lambda_i^+, \tilde{\varphi}^+ | i = 0, ..., 4\}$ and $\{\lambda_i^-, \tilde{\varphi}^- | i = 0, ..., 4\}$, where $\tilde{\varphi}^\pm = 2\pi - \varphi^\pm$ with $\pi \le \tilde{\varphi}^\pm \le 2\pi$. A state with $\{\lambda_i^+, \varphi^+ | i = 0, ..., 4\}$ is LU-equivalent to a state with $\{\lambda_i^-, \tilde{\varphi}^- | i = 0, ..., 4\}$, while a state with $\{\lambda_i^-, \varphi^- | i = 0, ..., 4\}$ is LU-equivalent to a state with $\{\lambda_i^+, \tilde{\varphi}^+ | i = 0, ..., 4\}$ [66]. Therefore we can focus on two possible positive-decomposition coefficients $\{\lambda_i^+, \varphi^+ | i = 0, ..., 4\}$ and $\{\lambda_i^-, \varphi^- | i = 0, ..., 4\}$ for a set of $(C_{AB}, C_{AC}, C_{BC}, \tau_{ABC}, J_5)$.

Next, we prove that the entanglement charge Q_e eliminates the non-uniqueness and that two states are LU-equivalent if and only if the six parameters $(C_{AB}, C_{AC}, C_{BC}, \tau_{ABC}, J_5, Q_\mathrm{e})$ of the two states are equal to each other. If $Q_\mathrm{e} \ne 0$, we can determine one positive-decomposition coefficients and one negative-decomposition

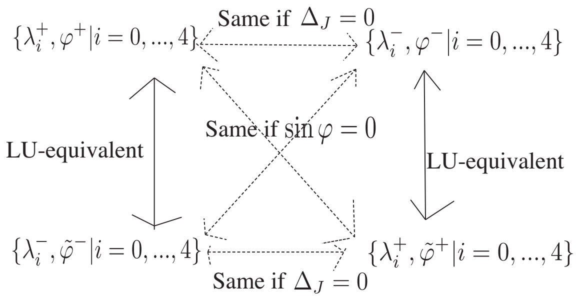

Figure B.4: The relation among the four sets of coefficients for $Q_{\rm e} = 0$. The relations indicated by solid lines are always valid, while those indicated by dotted lines are valid if and only if the noted conditions are satisfied.

coefficients uniquely from the parameters $(C_{AB}, C_{AC}, C_{BC}, \tau_{ABC}, J_5, Q_{\rm e})$ as follows:

$$\lambda_0^2 = \frac{J_5 + \tau_{ABC} \ddot{+} Q_{\rm e}\sqrt{\Delta_J}}{2(C_{BC}^2 + \tau_{ABC})} = \frac{K_5 \ddot{+} Q_{\rm e}\sqrt{\Delta_J}}{2K_{BC}}, \tag{B.27}$$

$$\lambda_2^2 = \frac{C_{AC}^2}{4\lambda_0^2}, \ \lambda_3^2 = \frac{C_{AB}^2}{4\lambda_0^2}, \ \lambda_4^2 = \frac{\tau_{ABC}}{4\lambda_0^2}, \tag{B.28}$$

$$\lambda_1^2 = 1 - \lambda_0^2 - \frac{C_{AB}^2 + C_{AC}^2 + \tau_{ABC}}{4\lambda_0^2}, \tag{B.29}$$

$$\cos\varphi = \frac{\lambda_1^2\lambda_4^2 + \lambda_2^2\lambda_3^2 - C_{BC}^2/4}{2\lambda_1\lambda_2\lambda_3\lambda_4}, \tag{B.30}$$

where $\ddot{+}$ is $+$ or $-$ when $\{\lambda_i, \varphi | i = 0, ..., 4\}$ are positive-decomposition coefficients or negative-decomposition coefficients, respectively. Thus, if $Q_{\rm e} \neq 0$, the set of $(C_{AB}, C_{AC}, C_{BC}, \tau_{ABC}, J_5)$ together with the entanglement charge $Q_{\rm e}$ gives a unique set of LU-equivalent states. Note that when $Q_e \neq 0$, the parameter $Q_{\rm e}$ is equal for the possible sets of coefficients of a state, because of (B.27)–(B.30).

If $Q_{\rm e} = 0$, at least one of $\sin\varphi$ and Δ_J is zero because of (B.6) and (B.22). If $\sin\varphi$ is zero, $\{\lambda_i^\pm, \varphi^\pm | i = 0, ..., 4\}$ and $\{\lambda_i^\pm, \tilde{\varphi}^\pm | i = 0, ..., 4\}$ are equal. If Δ_J is zero, $\{\lambda_i^+, \varphi^+ | i = 0, ..., 4\}$ and $\{\lambda_i^-, \varphi^- | i = 0, ..., 4\}$ are equal as $\{\lambda_i^+, \tilde{\varphi}^+ | i = 0, ..., 4\}$ and $\{\lambda_i^-, \tilde{\varphi}^- | i = 0, ..., 4\}$ are, respectively, because of (B.22). Thus, if $Q_{\rm e}$ is zero, the four sets of coefficients $\{\lambda_i^+, \varphi^+ | i = 0, ..., 4\}$, $\{\lambda_i^-, \varphi^- | i = 0, ..., 4\}$, $\{\lambda_i^+, \tilde{\varphi}^- | i = 0, ..., 4\}$ and $\{\lambda_i^-, \tilde{\varphi}^- | i = 0, ..., 4\}$ are LU-equivalent (Fig. B.4). Thus, if $Q_{\rm e} = 0$, the set of $(C_{AB}, C_{AC}, C_{BC}, \tau_{ABC}, J_5)$ gives a unique set of LU-equivalent states. Note that the above guarantees that when $Q_{\rm e} = 0$, the parameter $Q_{\rm e}$ is equal for the possible sets of coefficients of a state. Incidentally, a state is LU-equivalent to its complex-conjugate if and only if its entanglement charge $Q_{\rm e}$ is zero. The complex conjugate transformation of the state only changes the sign of φ. Thus, a state is LU-equivalent to its complex conjugate if and only if $\{\lambda_i^\pm, \varphi^\pm | i = 0, ..., 4\}$ are LU-equivalent to $\{\lambda_i^\pm, \tilde{\varphi}^\pm | i = 0, ..., 4\}$; this LU-equivalence is illustrated in Fig. B.4.

For the reasons stated above, the set of $(C_{AB}, C_{AC}, C_{BC}, \tau_{ABC}, J_5)$ together with the entanglement charge $Q_{\rm e}$ gives a unique set of LU-equivalent states. In other words, two states are LU-equivalent if and only if the C-parameters $(C_{AB}, C_{AC}, C_{BC}, \tau_{ABC}, J_5, Q_{\rm e})$ of the two states are equal to each other. This is the statement of Theorem 10, and thus the proof is completed. □

Note that a state is LU-equivalent to its complex conjugate if and only if $Q_{\rm e} = 0$. Thus, the condition $Q_{\rm e} = 0$ is equivalent to $E_6 = 0$ in Ref. [57].

B.3 The Proof of Theorem 11

In this section, we prove Theorem 11. All the deterministic LOCC transformations are categorized into any of the following cases determined by the initial and final states:

Case $\mathfrak{A}$: Both of the initial and final states are EP definite and the initial state is GHZ-type.

Case $\mathfrak{B}$: The initial state is EP definite and the final state is EP indefinite.

Case $\mathfrak{C}$: The initial state is EP indefinite and GHZ-type.

Case $\mathfrak{D}$: The tangle of initial state is zero.

Note that these four Cases exhaust all cases of the initial and final states; (*Proof*: The case where both the initial and final states are EP-definite is exhausted by Cases $\mathfrak{A}$, $\mathfrak{C}$ and $\mathfrak{D}$. The case where the initial state is EP-definite and the final state is EP-indefinite is Case $\mathfrak{B}$. The case where the initial state is EP-indefinite is exhausted by Cases $\mathfrak{C}$ and $\mathfrak{D}$.$\square$)

We carry out the proof of each Case in sections B.3.1–B.3.4, respectively.

B.3.1 Case $\mathfrak{A}$

First, we prove Theorem 11 in Case $\mathfrak{A}$, where both of the initial and final states are EP definite and the initial state is GHZ-type. We will argue that we can assume the final state to be GHZ-type too. The final state after an LOCC transformation is EP definite, and hence the final state is a truly multipartite state. We cannot reach a W-type state from a GHZ-type initial state with an LOCC transformation [67]. Thus the final state must be GHZ-type. We can also show that if the initial and final states satisfy the two conditions of Theorem 11, the final state must be GHZ-type. (*Proof*: If the final state would not be GHZ-type, then τ'_{ABC} would be zero, and thus at least one of ζ, ζ_A, ζ_B and ζ_C would be zero. Then, at least one of K'_{AB}, K'_{AC} and K'_{BC} would be zero. Because of $K'_{\text{ap}} \geq J'_{\text{ap}}$, the final state would not be W-type. An EP-definite state is GHZ-type or W-type, and thus this is a contradiction. $\square$) Thus, in the present case, we only have to consider the case in which both initial and final states are GHZ-type. In this case, a necessary and sufficient condition of the possibility of a d-LOCC transformation is already given [68]. Thus, in the present case, we only have to prove the equivalence between the conditions of Theorem 11 and the necessary and sufficient condition.

An arbitrary GHZ-type state can be expressed as follows [68]:

$$|\psi\rangle = \frac{1}{\sqrt{N}}(|\tilde{0}_A\tilde{0}_B\tilde{0}_C\rangle + z\,|\tilde{1}_A\tilde{1}_B\tilde{1}_C\rangle), \tag{B.31}$$

where $\{|\tilde{0}_i\rangle\,|i = A, B, C\}$ and $\{|\tilde{1}_i\rangle\,|i = A, B, C\}$ are normalized states of the qubits A, B and C, with their relative phases adjusted such that all of $c_i \equiv \langle\tilde{0}_i|\tilde{1}_i\rangle$ are real and non-negative, while z is an arbitrary complex number and N is the normalization constant. There are two possible expressions of the form (B.31) for an arbitrary state. These two expressions have the same values of $\{c_i\}$ but different values of z. The relation between the two values of z is as follows:

$$\text{If there is no zeros in the set } \{c_i\}: \quad z_1 = \frac{1}{z_2}, \tag{B.32}$$

$$\text{If there is a zero in the set } \{c_i\}: \quad |z_1| = \frac{1}{|z_2|}, \tag{B.33}$$

where z_1 and z_2 are the values of z in the two possible expressions of the form (B.31).

When the set $\{c_i\}$ of the states $|\psi\rangle$ and the set $\{c_i'\}$ of $|\psi'\rangle$ have no zeros, a d-LOCC transformation from the state $|\psi\rangle$ to the state $|\psi'\rangle$ is executable if and only if the following expressions are satisfied [68]:

$$c_i' \geq c_i \ \ (k = A, B, C), \tag{B.34}$$
$$\frac{s'}{s} = \frac{c_A c_B c_C}{c_A' c_B' c_C'}, \tag{B.35}$$
$$\frac{n'}{n} = \frac{c_A c_B c_C}{c_A' c_B' c_C'}, \tag{B.36}$$

where

$$n \equiv \frac{2\mathrm{Re}[z]}{|z|^2+1}, \ \ s \equiv \frac{2\mathrm{Im}[z]}{|z|^2-1} \tag{B.37}$$

with the parameter z of the state $|\psi\rangle$, and s' and n' are defined for the state $|\psi'\rangle$ with the parameter z'. The parameter z can take the two different values, but n and s have the same values for each value of z, except for $z = \pm 1$; when $(|z| = 1) \wedge (z \neq \pm 1)$, we consider the parameter s to take one value ∞. In the case where $z = \pm 1$, the parameter s becomes indefinite; it becomes $0/0$. When the parameter s becomes indefinite, we only leave out (B.35). The parameter s is indefinite if and only if $z = \pm 1$. As we will show later, the equation $z = \pm 1$ is equivalent to (B.14) in Theorem 11. There are two other cases where we have to treat (B.35) and (B.36) exceptionally; the case where at least one of s and s' becomes 0 or ∞, and the case where at least one of n and n' becomes 0. In the former case, we consider that (B.35) holds if and only if s and s' has the same value; for example, if s takes ∞, the equation (B.35) holds if and only if $s' = \infty$. In the same manner, in the latter case, we consider that (B.36) holds if and only if n and n' has the same value.

Let us prove that (B.34)–(B.36) are equivalent to the conditions of Theorem 11. We can express the paramters z and $\{c_i\}$ in terms of the C-paramters:

$$z = -\frac{\sqrt{K_{AB}K_{AC}}}{2\lambda_0^2\sqrt{K_{BC}}}e^{-i\tilde{\varphi}_5}, \tag{B.38}$$
$$c_A = \frac{C_{BC}}{\sqrt{K_{BC}}}, \ \ c_B = \frac{C_{AC}}{\sqrt{K_{AC}}}, \ \ c_C = \frac{C_{AB}}{\sqrt{K_{AB}}}, \tag{B.39}$$

where

$$e^{-i\tilde{\varphi}_5} = \frac{\lambda_2\lambda_3 - \lambda_1\lambda_4 e^{i\varphi}}{|\lambda_2\lambda_3 - \lambda_1\lambda_4 e^{i\varphi}|} = \cos\varphi_5 - i\mathrm{sgn}[\sin\varphi]\sin\varphi_5. \tag{B.40}$$

Because there are two possible sets of $\{\lambda_i, \varphi | i = 0, ..., 4\}$ in (B.38), the parameter z takes two values, which are z_1 and z_2 in (B.32) and (B.33). The derivation of the above expressions is given in Appendix B. It is easily seen from (B.39) that the set $\{c_i\}$ of a state has no zeros if and only if the state is EP-definite. Now that we have reduced Case $\mathfrak{A}$ into the case in which the initial and final states are EP-definite and GHZ-type, we only have to prove that (B.34)–(B.36) are equivalent to the conditions of Theorem 11.

Using (B.38) and (B.39), we prove that (B.34) and (B.36) are equivalent to the condition 1 of Theorem 11 except for $\zeta_{\mathrm{lower}} \leq \zeta \leq 1$. Substituting (B.39) into (B.34), we transform (B.34) into

$$\frac{\tau_{ABC}'}{\tau_{ABC}} \leq \frac{K_{AB}'}{K_{AB}}, \ \ \frac{\tau_{ABC}'}{\tau_{ABC}} \leq \frac{K_{AC}'}{K_{AC}}, \ \ \frac{\tau_{ABC}'}{\tau_{ABC}} \leq \frac{K_{BC}'}{K_{BC}}. \tag{B.41}$$

Because of (B.40),

$$\mathrm{Re}[z] = -\frac{\sqrt{K_{AB}K_{AC}}}{2\lambda_0^2\sqrt{K_{BC}}}\cos\varphi_5. \tag{B.42}$$

Because the possible two sets of $\{\lambda_i, \varphi | i = 0, ..., 1\}$ are $\{\lambda_i^+, \varphi^+ | i = 0, ..., 1\}$ and $\{\lambda_i^-, \tilde{\varphi}^- | i = 0, ..., 1\}$ or $\{\lambda_i^-, \varphi^- | i = 0, ..., 1\}$ and $\{\lambda_i^+, \tilde{\varphi}^+ | i = 0, ..., 1\}$, we obtain

$$n = -\frac{\sqrt{K\mathrm{ap}}}{2K_5}\cos\varphi_5. \tag{B.43}$$

Thus, we can trasform (B.36) into

$$\frac{K_5'}{K_5} = \frac{J_5'}{J_5} \text{ (for } n \neq 0), \quad J_5 = J_5' = 0 \text{ (for } n = 0). \tag{B.44}$$

Let us then prove that the expressions (B.41) and (B.44) are equivalent to the existence of $0 \leq \zeta \leq 1$, $0 \leq \zeta_A \leq 1$, $0 \leq \zeta_B \leq 1$ and $0 \leq \zeta_C \leq 1$, which satisfy (B.12). To show this, we only have to define ζ, ζ_A, ζ_B and ζ_C as follows:

$$\zeta_A = \frac{K_{BC}\tau'_{ABC}}{K'_{BC}\tau_{ABC}}, \ \zeta_B = \frac{K_{AC}\tau'_{ABC}}{K'_{AC}\tau_{ABC}}, \ \zeta_C = \frac{K_{ABf}\tau'_{ABC}}{K'_{AB}\tau_{ABC}}, \tag{B.45}$$

$$\zeta = \frac{\tau'_{ABC}}{\tau_{ABC}\zeta_A\zeta_B\zeta_C}. \tag{B.46}$$

Because of (B.44), (B.45) and (B.46), the parameters ζ, ζ_A, ζ_B and ζ_C satisfy (B.12). Because of (B.41), the parameters ζ_A, ζ_B and ζ_C are less than or equal to one. Because of (B.45) and (B.46), the parameters ζ_A, ζ_B and ζ_C are greater than or equal to zero. Thus, the expressions (B.34) and (B.36) are equivalent to the condition 1 of Theorem 11, except for $\zeta_{\mathrm{lower}} \leq \zeta \leq 1$.

Now we have proven that the equations (B.34) and (B.36), which are the ones on the parameters $\{c_i\}$ and n, are equivalent to the condition 1 of Theorem 11 except for $\zeta_{\mathrm{lower}} \leq \zeta \leq 1$. Next, let us prove that the condition on the parameter s is equivalent to the inequality $\zeta_{\mathrm{lower}} \leq \zeta \leq 1$ and the condition 2 of Theorem 11. Hereafter, we assume the condition 1 of Theorem 11 except for $\zeta_{\mathrm{lower}} \leq \zeta \leq 1$ until the end of Case $\mathfrak{A}$. The condition on s is (B.35) for $z \neq \pm 1$ but is left out for $z = \pm 1$. First, we prove that the equation $z = \pm 1$ is equivalent to (B.14). Because of (B.38), we can transform $z = \pm 1$ into

$$z = \pm 1 \quad \Leftrightarrow \quad (\tilde{\varphi}_5 = 0, \pi) \wedge \left(\frac{\sqrt{K_{AB}K_{AC}}}{2\lambda_0^2\sqrt{K_{BC}}} = 1\right) \tag{B.47}$$

$$\Leftrightarrow \quad (J\mathrm{ap}\sin^2\varphi_5 = 0) \wedge \left(\frac{\sqrt{K\mathrm{ap}}}{K_5 \pm \sqrt{\Delta_J}} = 1\right) \tag{B.48}$$

$$\Leftrightarrow \quad (J\mathrm{ap}\sin^2\varphi_5 = 0) \wedge (\Delta_J = 0) \tag{B.49}$$

$$\Leftrightarrow \quad (J\mathrm{ap} - J_5^2 = 0) \wedge (\Delta_J = 0). \tag{B.50}$$

where the double sign $\pm$ in (B.48) is the one in (B.22); note that the possible two sets of $\{\lambda_i, \varphi | i = 0, ..., 1\}$ are $\{\lambda_i^+, \varphi^+ | i = 0, ..., 1\}$ and $\{\lambda_i^-, \tilde{\varphi}^- | i = 0, ..., 1\}$ or $\{\lambda_i^-, \varphi^- | i = 0, ..., 1\}$ and $\{\lambda_i^+, \tilde{\varphi}^+ | i = 0, ..., 1\}$.

Thus, the equation $z = \pm 1$ is equivalent to (B.14). In other words, Eq. (B.14) does not hold for $z \neq \pm 1$.

Let us next prove that the condition on s is equivalent to the condition 2 of Theorem 11 and $\zeta_{\mathrm{lower}} \leq \zeta \leq 1$ in the case $z \neq \pm 1$. In this case, what we have to prove is that (B.35) is equivalent to the condition 2 of Theorem

11 and $\zeta_{\rm lower} \le \zeta \le 1$. In this case, (B.14) does not hold, and thus $|\psi\rangle$ is $\tilde{\zeta}$-definite. Hence, we only have to prove that (B.35) is equivalent to (B.15). (Note that $\zeta_{\rm lower} \le \tilde{\zeta} \le 1$.) To prove the equivalence of (B.35) and (B.15), we first express s in terms of the K-parameters. When $Q_{\rm e} \neq 0$, by substituting (B.27) and (B.40) into (B.35), we obtain

$$s = -\frac{\sqrt{K_{\rm ap}}}{Q_{\rm e}\sqrt{\Delta_J}} \sin\varphi_5. \tag{B.51}$$

Because of (B.39) and (B.51),

$$\frac{Q'_{\rm e}\sqrt{\Delta_J}}{Q_{\rm e}\sqrt{\Delta'_J}} \frac{\sqrt{J'_{\rm ap}}\sin\varphi'_5}{\sqrt{J_{\rm ap}}\sin\varphi_5} = 1 \tag{B.52}$$

always holds. Substituting $\Delta_J = K_5^2 - K_{\rm ap}$, $J_{\rm ap}\sin^2\varphi_5 = J_{\rm ap} - J_5^2$ and (B.12) into (B.52) and reducing it, we can obtain $Q_{\rm e} = Q'_{\rm e}$ and $\zeta = \tilde{\zeta}$. Thus, when $Q_{\rm e} \neq 0$, (B.15) is equivalent to (B.35).

Now we consider the case where $z \neq \pm 1$, and thus when $Q_{\rm e} = 0$, only one of the expressions $\sin\varphi_5 = 0$ and $\Delta_J = 0$ holds. When $\sin\varphi_5 = 0$ holds, the equation (B.35) is equivalent to $s = s' = 0$. When $\Delta_J = 0$ holds, the equation (B.35) is equivalent to $s = s' = \infty$. Because of (B.37) and (B.38), the equations $s = s' = 0$ and $s = s' = \infty$ are equivalent to $\sin\varphi_5 = \sin\varphi'_5 = 0$ and $\Delta_J = \Delta'_J = 0$, respectively. Because of $(Q_{\rm e} = 0) \Leftrightarrow ((\sin\varphi_5 = 0) \vee (\Delta_J = 0))$, $\Delta_J = K_5^2 - K_{\rm ap}$, $J_{\rm ap}\sin^2\varphi_5 = J_{\rm ap} - J_5^2$ and (B.12), when the equation $\sin\varphi_5 = 0$ holds, the equation $\sin\varphi_5 = \sin\varphi'_5 = 0$ is equivalent to (B.15). In the same manner, when the equation $\Delta_J = 0$ holds, $\Delta_J = \Delta'_J = 0$ is equivalent to (B.15). Thus, when $Q_{\rm e} = 0$, the expression (B.15) is equivalent to (B.35). We have already proven that when $Q_{\rm e} \neq 0$, the expression (B.15) is equivalent to (B.35). Thus, (B.15) is equivalent to (B.35).

Finally, we consider the case $z = \pm 1$. In this case, there is no condition of s and the condition (B.14) holds. Because of (B.14), the condition 2 of Theorem 11 becomes (B.17) in this case. Thus, we only have to prove that (B.14) is equivalent to $\zeta_{\rm lower} \le \zeta \le 1$ and (B.17). Because we have assumed the condition 1 of Theorem 10 except for $\zeta_{\rm lower} \le \zeta \le 1$, we obtain the following equations:

$$\frac{J_5'^2}{J'_{\rm ap}} = \frac{\zeta_{\rm lower}}{\zeta}\frac{J_5^2}{J_{\rm ap}}, \tag{B.53}$$

$$\Delta'_J = (\zeta\zeta_A\zeta_B\zeta_C)^2(K_5^2 - \zeta K_{\rm ap}) \ge (\zeta\zeta_A\zeta_B\zeta_C)^2\Delta_J. \tag{B.54}$$

The derivation of (B.53) and (B.54) is as follows:

$$\begin{aligned} \frac{J_5'^2}{J'_{\rm ap}} &= \frac{(\zeta\zeta_A\zeta_B\zeta_C)^2 J_5^2}{\zeta^3\zeta_A^2\zeta_B^2\zeta_C^2(K_{BC} - \zeta_A\tau_{ABC})(K_{AC} - \zeta_B\tau_{ABC})(K_{AB} - \zeta_C\tau_{ABC})} \\ &= \frac{\zeta_{\rm lower}}{\zeta}\frac{J_5^2}{J_{\rm ap}}, \end{aligned} \tag{B.55}$$

$$\begin{aligned} \Delta'_J &= (\zeta\zeta_A\zeta_B\zeta_C)^2 K_5^2 - \zeta^3\zeta_A^2\zeta_B^2\zeta_C^2 K_{\rm ap} \\ &= (\zeta\zeta_A\zeta_B\zeta_C)^2(K_5^2 - \zeta K_{\rm ap}) \ge (\zeta\zeta_A\zeta_B\zeta_C)^2\Delta_J. \end{aligned} \tag{B.56}$$

By using (B.53) and (B.54), let us prove that (B.14) is equivalent to $\zeta_{\rm lower} \le \zeta \le 1$ and (B.17). First, we prove that (B.14) is a sufficient condition of $\zeta_{\rm lower} \le \zeta \le 1$ and (B.17) When (B.14) is valid, the equation $J_5^2/J_{\rm ap} = 1$ holds. Because $J_5'^2/J'_{\rm ap} = \cos^2\varphi'_5 \le 1$ is always valid, when (B.14) is valid, the inequality $\zeta_{\rm lower} \le \zeta$ follows (B.53). In the same manner, when (B.14) is valid, the inequality $\zeta \le 1$ follows (B.54). Then, note that the equation $J_5'^2 = J'_{\rm ap}$ holds if and only if $\zeta = \zeta_{\rm lower}$ holds, and that the equation $\Delta'_J = 0$ holds if and only if $\zeta = 1$ holds. Because of (B.6), the equation $Q'_{\rm e} = 0$ holds if and only if $(\Delta'_J = 0) \vee (J'^2_5 = J'_{\rm ap})$ holds. Thus, when (B.14) is valid, $Q'_{\rm e} = 0$ if and only if $\zeta = \zeta_{\rm lower}$ or $\zeta = 1$. In the other words, now we have proven that (B.14) is a sufficient condition of $\zeta_{\rm lower} \leq \zeta \leq 1$ and (B.17).

Let us prove that (B.14) is also a necessary condition. Because of $\zeta_{\rm lower} \leq \zeta \leq 1$, (B.53), (B.54) and (B.6), the equation $|Q'_{\rm e}| = {\rm sgn}[(1-\zeta)(\zeta - \zeta_{\rm lower})]$ is valid if and only if both of Δ_J and $J_5^2 - J_{\rm ap}$ are zero. In the other words, (B.14) is also a necessary condition of $\zeta_{\rm lower} \leq \zeta \leq 1$ and (B.17). Thus, (B.14) is equivalent to $\zeta_{\rm lower} \leq \zeta \leq 1$ and (B.17), and thus we have completed the proof in Case $\mathfrak{A}$. □

B.3.2 Case $\mathfrak{B}$

In this subsection, we prove Theorem 11 in Case $\mathfrak{B}$, where the initial state is EP-definite and the final state is EP-indefinite. In the proof, we will use the following two lemmas which describe how a measurement changes entanglement.

Lemma 16. *Let us consider the situation where a measurement $\{M_{(i)}\}$ is performed on the qubit A of an arbitrary three-qubit state $|\psi\rangle$. The state $\left|\psi^{(i)}\right\rangle \equiv M_{(i)} |\psi\rangle / \sqrt{p_{(i)}}$ is obtained as the i-th result with the probability $p_{(i)}$. Then, the following equations are valid:*

$$C_{AB}^{(i)} = \alpha^{(i)} C_{AB}, \ \ C_{AC}^{(i)} = \alpha^{(i)} C_{AC}, \ \ \sqrt{\tau_{ABC}^{(i)}} = \alpha^{(i)} \sqrt{\tau_{ABC}}, \tag{B.57}$$

$$p_{(i)} C_{BC}^{(i)} = |k_{(i)} \sqrt{\tau_{ABC}} e^{i(\theta_{(i)} + \tilde{\varphi}_5)} - C_{BC} b_{(i)}|, \tag{B.58}$$

$$p_{(i)} = \lambda_0^2 a_{(i)} + (1-\lambda_0^2) b_{(i)} + 2\lambda_0\lambda_1 k_{(i)} \cos(\theta_{(i)} - \varphi). \tag{B.59}$$

where $C_{AB}^{(i)}$, $C_{AC}^{(i)}$, $C_{BC}^{(i)}$ and $\tau_{ABC}^{(i)}$ are the concurrences and the tangle of the state $\left|\psi^{(i)}\right\rangle$ and

$$M_{(i)}^\dagger M_{(i)} \equiv \begin{pmatrix} a_{(i)} & k_{(i)} e^{-i\theta_{(i)}} \\ k_{(i)} e^{i\theta_{(i)}} & b_{(i)} \end{pmatrix}, \tag{B.60}$$

$$a_{(i)} b_{(i)} - k_{(i)}^2 \geq 0, \ \ a_{(i)} \geq 0, \ \ b_{(i)} \geq 0, \ \ k_{(i)} \geq 0, \ \ 0 \leq \theta_{(i)} \leq 2\pi, \tag{B.61}$$

$$\alpha^{(i)} \equiv \frac{\sqrt{a_{(i)} b_{(i)} - k_{(i)}^2}}{p_{(i)}}. \tag{B.62}$$

Proof: When we perform a transformation which is expressed as

$$M = \begin{pmatrix} M_{00} & M_{01} \\ M_{10} & M_{11} \end{pmatrix}, \qquad M_{00}, M_{01}, M_{10}, M_{11} \in \mathbb{C}, \tag{B.63}$$

on the qubit A of a pure state (B.1), the state $|\psi\rangle$ is transformed into

$$\begin{aligned} M|\psi\rangle = (\lambda_0 M_{00} |0\rangle + \lambda_0 M_{10} |1\rangle + \lambda_1 e^{i\varphi} M_{01} |0\rangle + \lambda_1 e^{i\varphi} M_{11} |1\rangle) |00\rangle \\ + \lambda_2 (M_{01}|0\rangle + M_{11}|1\rangle)|01\rangle + \lambda_3 (M_{01}|0\rangle + M_{11}|1\rangle)|10\rangle + \lambda_4 (M_{01}|0\rangle + M_{11}|1\rangle)|11\rangle. \end{aligned} \tag{B.64}$$

We can transform (B.64) into the form of the generalized Schmidt decomposition (B.1) with straightforward algebra;

$$M|\psi\rangle = \frac{\lambda_0 \det\sqrt{M^\dagger M}}{\sqrt{|M_{01}|^2+|M_{11}|^2}}|000\rangle + \frac{\lambda_0(M_{00}M_{01}^* + M_{10}M_{11}^*) + \lambda_1 e^{i\varphi}(|M_{01}|^2+|M_{11}|^2)}{\sqrt{|M_{01}|^2+|M_{11}|^2}}|100\rangle + \sqrt{|M_{01}|^2+|M_{11}|^2}(\lambda_2|101\rangle + \lambda_3|110\rangle + \lambda_4|111\rangle). \quad (B.65)$$

Note that each coefficient of the generalized Schmidt decomposition (B.65) of $M|\psi\rangle$ above is expressed by the components of $M^\dagger M$ solely:

$$M^\dagger M = \begin{pmatrix} |M_{00}|^2+|M_{10}|^2 & M_{00}^*M_{01}+M_{10}^*M_{11} \\ M_{01}^*M_{00}+M_{11}^*M_{10} & |M_{01}|^2+|M_{11}|^2 \end{pmatrix}. \quad (B.66)$$

Then expressing the components of $M_{(i)}^\dagger M_{(i)}$ as in (B.60), we can also express $M_{(i)}|\psi\rangle$ and $p_{(i)}$ as

$$M_{(i)}|\psi\rangle = \frac{\lambda_0\sqrt{a_{(i)}b_{(i)}-k_{(i)}^2}}{\sqrt{b_{(i)}}}|000\rangle + \frac{\lambda_0 k_{(i)}e^{i\theta_{(i)}} + \lambda_1 e^{i\varphi}b_{(i)}}{\sqrt{b}_{(i)}}|100\rangle + \lambda_2\sqrt{b_{(i)}}|101\rangle + \lambda_3\sqrt{b_{(i)}}|110\rangle + \lambda_4\sqrt{b_{(i)}}|111\rangle. \quad (B.67)$$

$$\begin{aligned} p_{(i)} &= \langle\psi| M_{(i)}^\dagger M_{(i)}|\psi\rangle \\ &= \lambda_0^2 a_{(i)} + (1-\lambda_0^2)b_{(i)} + 2\lambda_0\lambda_1 k_{(i)}\cos(\theta_{(i)}-\varphi). \end{aligned} \quad (B.68)$$

Because of $\left|\psi^{(i)}\right\rangle = M_{(i)}|\psi\rangle/\sqrt{p_{(i)}}$, we can express the coefficients of the generalized Schmidt decomposition $\{\lambda^{(i)}|k=0,...,4\}$ as

$$\lambda_0^{(i)} = \frac{\lambda_0\sqrt{a_{(i)}b_{(i)}-k_{(i)}^2}}{\sqrt{p_{(i)}}\sqrt{b_{(i)}}}, \quad (B.69)$$

$$\lambda_1^{(i)}e^{i\varphi^{(i)}} = \frac{\lambda_0 k_{(i)}e^{i\theta_{(i)}} + \lambda_1 e^{i\varphi}b_{(i)}}{\sqrt{p_{(i)}}\sqrt{b_{(i)}}}, \quad (B.70)$$

$$\lambda_2^{(i)} = \frac{\lambda_2\sqrt{b_{(i)}}}{\sqrt{p_{(i)}}},\ \lambda_3^{(i)} = \frac{\lambda_3\sqrt{b_{(i)}}}{\sqrt{p_{(i)}}},\ \lambda_4^{(i)} = \frac{\lambda_4\sqrt{b_{(i)}}}{\sqrt{p_{(i)}}}. \quad (B.71)$$

Because of (B.2), (B.3) and (B.69)–(B.71), the equations (B.57) and (B.58) are valid. □

Lemma 17. *Let the notation $\{M_{(i)}|i=1,2\}$ stand for an arbitrary two-choice measurement which is operated on the qubit A of a three-qubit pure state $|\psi_{ABC}\rangle$. We refer to each result of the measurements $\{M_{(i)}|i=1,2\}$ as $\left|\psi_{ABC}^{(i)}\right\rangle$. Let the notations ($C_{AB}$,$C_{AC}$,$C_{BC}$,$\tau_{ABC}$,$J_5$,$Q_e$) and ($C_{AB}^{(i)}$,$C_{AC}^{(i)}$,$C_{BC}^{(i)}$,$\tau_{ABC}^{(i)}$,$J_5^{(i)}$,$Q_e^{(i)}$) stand for the sets of the C-parameters of the states $|\psi_{ABC}\rangle$ and $\left|\psi_{ABC}^{(i)}\right\rangle$, respectively. Then, the following inequalities hold:*

$$C_{BC} \le \sum_{i=0}^{1} p_{(i)}C_{BC}^{(i)} \le \sqrt{C_{BC}^2 + \left[1-\left(\sum_{k=0}^{1}p_{(i)}\alpha^{(i)}\right)^2\right]\tau_{ABC}}, \quad (B.72)$$

where the probability $p_{(i)}$ and the multiplication factor $\alpha^{(i)}$ are defined in (B.59) *and* (B.62), *respectively.*

Proof: The average $\sum_{i=0}^{1}p_{(i)}C_{BC}^{(i)}$ is equal to the length of the heavy line in Fig. B.5, because we can

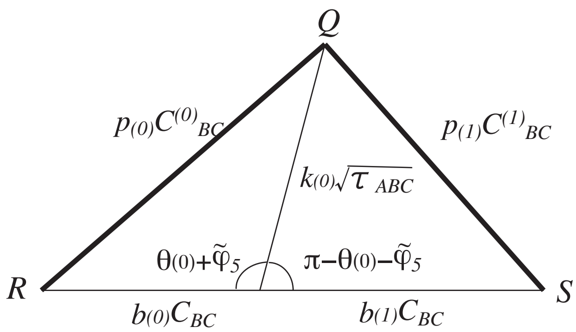

Figure B.5: A geometric interpretation of the change of C_{BC}.

interpret (B.58) as the cosine theorem and because $b_{(0)} + b_{(1)} = 1$ and $\sum_i \vec{k}_{(i)} = 0$. The end points of the heavy line have to coincide with the end points of the segment RS because $\sum_i \vec{k}_{(i)} = 0$. Then, the left inequality $C_{BC} \leq \sum_{i=1}^{2} p_i C_{BC}^{(i)}$ clearly holds, since a polygonal line is longer than a straight line.

To prove the right inequality of this Lemma, it suffices to show the inequality

$$\begin{aligned} &\sqrt{(bC_{BC} + k\cos\theta\sqrt{\tau_{ABC}})^2 + (k\sin\theta\sqrt{\tau_{ABC}})^2} \\ &+\sqrt{[(1-b)C_{BC} - k\cos\theta\sqrt{\tau_{ABC}}]^2 + (k\sin\theta\sqrt{\tau_{ABC}})^2} \\ &\leq \sqrt{C_{BC}^2 + \{1 - [\sqrt{ab-k^2} + \sqrt{(1-a)(1-b)-k^2}]^2\}\tau_{ABC}} \end{aligned} \tag{B.73}$$

under the conditions $ab - k^2 \geq 0$, $(1-a)(1-b) - k^2 \geq 0$, $0 \leq \theta \leq 2\pi$, $0 \leq a \leq 1$ and $0 \leq b \leq 1$, where we used the substitutions:

$$a_{(0)} = a,\ \ a_{(1)} = 1-a,\ \ b_{(0)} = b,\ \ b_{(1)} = 1-b,\ \ \theta_{(0)} + \tilde{\varphi}_5 = \pi - \theta. \tag{B.74}$$

The fact that θ can take any value guarantees the last substitution.

Let us find maximum value of the left-hand side of (B.73) with the values of the measurement parameters a, b and k fixed. We can express the left-hand side of (B.73) as

$$\sqrt{u^2 + w^2 + 2uw\cos\theta} + \sqrt{v^2 + w^2 - 2vw\cos\theta}, \tag{B.75}$$

where $u = bC_{BC}$, $v = (1-b)C_{BC}$ and $w = k\sqrt{\tau_{ABC}}$. With the values of u, v and w fixed, the quantity (B.75) is maximized to be $(u+v)\sqrt{1 + w^2/(uv)}$ at the point $\cos\theta = w(u-v)/2uv$. Substituting $u = bC_{BC}$, $v = (1-b)C_{BC}$ and $w = k\sqrt{\tau_{ABC}}$ give that

$$\text{the maximum of the left-hand side of (B.73)} = \sqrt{C_{BC}^2 + \frac{k^2\tau_{ABC}}{b(1-b)}}. \tag{B.76}$$

Hence, in order to prove Lemma 17, it suffices to show

$$\frac{k^2}{b(1-b)} \leq 1 - [\sqrt{ab-k^2} + \sqrt{(1-a)(1-b)-k^2}]^2. \tag{B.77}$$

After straightforward algebra, (B.77) is reduced to

$$\left[(a-b)+k^2\frac{(b^2-(1-b)^2)}{b(1-b)}\right]^2 \geq 0. \tag{B.78}$$

Hence we have proved the right inequality of (B.72) and thereby completed the proof of Lemma 17.□

Note that Lemma has the following corollary:

$$0 \leq \sum_i p_{(i)}\alpha_i \leq 1. \tag{B.79}$$

Now we have completed the preparation. Let us start the proof of Theorem 11 in Case $\mathfrak{B}$. In the present Case, the final state is EP-indefinite, and thus we can neglect the condition 2 of Theorem 11. Thus, we only have to show that the condition 1 of Theorem 10 is a necessary and sufficient condition of the possibility of a d-LOCC transformation.

Let us prove that a d-LOCC transformation from $|\psi\rangle$ to $|\psi'\rangle$ is executable if $|\psi\rangle$ and $|\psi'\rangle$ satisfy the condition 1 of Theorem 11. First we prove that if $|\psi\rangle$ and $|\psi'\rangle$ satisfy the condition 1 of Theorem 11, the state $|\psi'\rangle$ is biseparable or full-separable. Because $|\psi\rangle$ is EP-definite and because of (B.9),

$$K_{AB} > \tau_{ABC},\ \ K_{AB} > \tau_{ABC},\ \ K_{BC} > \tau_{ABC}. \tag{B.80}$$

Because $|\psi'\rangle$ is EP-indefinite, at least one of

$$K'_{AB} = \tau'_{ABC},\ \ K'_{AB} = \tau'_{ABC},\ \ K'_{BC} = \tau'_{ABC} \tag{B.81}$$

holds. We can assume $K'_{AB} = \tau'_{ABC}$ without losing generality. Because of (B.80), $K'_{AB} = \tau'_{ABC}$ and the condition 1 of Theorem 11, at least one of ζ, ζ_A, ζ_B is zero. When only one of ζ_A and ζ_B is zero and ζ is not zero, the state $|\psi'\rangle$ is biseparable; only K'_{BC} or K'_{AC} is not zero. When both of ζ_A and ζ_B are zero or ζ is zero, the state $|\psi'\rangle$ is full-separable; all of the K-parameters of $|\psi'\rangle$ are zero. Now we have proven that if $|\psi\rangle$ and $|\psi'\rangle$ satisfy the condition 1 of Theorem 11, the state $|\psi'\rangle$ is biseparable or full-separable.

Next, let us prove that if $|\psi\rangle$ and $|\psi'\rangle$ satisfy the condition 1 of Theorem 11, there is an executable d-LOCC transformation from $|\psi\rangle$ to $|\psi'\rangle$. Now the state $|\psi'\rangle$ is biseparable or full-separable. Without losing generality, we can assume that C'_{BC} is the only nonzero parameter in $(C'_{AB}, C'_{AC}, C'_{BC}, \tau'_{ABC}, J'_5, Q'_{\mathrm{e}})$. Because $|\psi\rangle$ and $|\psi'\rangle$ satisfy the condition 1 of Theorem 11, the inequality $C'^2_{BC} \leq K_{BC}$ holds. The set of full-separable states and biseparable states which have the same kind of bipartite entanglement is a totally ordered set [69]. In other words, when two states $|\psi\rangle$ and $|\psi'\rangle$ belong to such a set, there is an executable deterministic LOCC transformation from the EP-definite state $|\psi\rangle$ to the EP-indefinite state $|\psi'\rangle$ if and only if the bipartite entanglement of the state $|\psi\rangle$ is greater than or equal to that of the state $|\psi'\rangle$. Thus, if there is the following measurement $\{M_{(i)}\}$, there is an executable d-LOCC transformation from $|\psi\rangle$ to $|\psi'\rangle$; a measurement whose results can be transformed into a unique state $|\psi''\rangle$ by local unitary operations without exception, where $|\psi''\rangle$ is a biseparable state whose C^2_{BC} is equal to K_{BC} of $|\psi\rangle$. The measurement $\{M_{(i)}\}$ is given as follows:

$$M^\dagger_{(0)}M_{(0)} = \begin{pmatrix} a_{(0)} & k_{(0)}e^{-i\theta_{(0)}} \\ k_{(0)}e^{i\theta_{(0)}} & b_{(0)} \end{pmatrix} = \begin{pmatrix} a & ke^{-i\theta} \\ ke^{i\theta} & b \end{pmatrix}, \tag{B.82}$$

$$M_{(1)}^{\dagger} M_{(1)} = \begin{pmatrix} a_{(1)} & k_{(1)} e^{-i\theta_{(1)}} \\ k_{(1)} e^{i\theta_{(1)}} & b_{(1)} \end{pmatrix} = \begin{pmatrix} 1-a & -ke^{-i\theta} \\ -ke^{i\theta} & 1-b \end{pmatrix}, \tag{B.83}$$

where the measurement parameters a, b, k and θ are defined as follows:

$$a = \frac{1}{2} - \frac{\lambda_1 \sin\varphi}{2\sqrt{\lambda_1^2 \sin^2\varphi + \lambda_0^2}}, \tag{B.84}$$

$$b = \frac{1}{2} + \frac{\lambda_1 \sin\varphi}{2\sqrt{\lambda_1^2 \sin^2\varphi + \lambda_0^2}}, \tag{B.85}$$

$$k = \frac{\lambda_0}{2\sqrt{\lambda_1^2 \sin^2\varphi + \lambda_0^2}}, \tag{B.86}$$

$$\theta = \frac{\pi}{2}. \tag{B.87}$$

With substituting (B.84)–(B.87) into (B.57) and (B.58) and after straightforward algebra, we can confirm that the measurement $\{M_{(i)}\}$ is the measurement that we sought. Thus, we have proven that the condition 1 of Theorem 11 is a sufficient condition for the existence of an executable d-LOCC transformation.

Next, let us prove that the condition 1 of Theorem 11 is also a necessary condition. In other words, we prove that if there is an executable d-LOCC transformation from $|\psi\rangle$ to $|\psi'\rangle$, the states $|\psi\rangle$ and $|\psi'\rangle$ must satisfy the condition 1 of Theorem 11. It is possible to substitute two-choice measurements for any measurements of an LOCC transformation on a three-qubit pure state [67]. Hereafter, unless specified otherwise, measurements of LOCC transformations will be two-choice measurements. First, we prove that a deterministic LOCC transformation from an EP-definite state to an EP-indefinite state is executable only if the final state is biseparable or full-separable. We prove Lemma 18, which generally holds for stochastic LOCC transformation including d-LOCC transformations.

Lemma 18. *Let the notation T_{SL} stand for an LOCC transformation from an arbitrary EP-definite state $|\psi\rangle$ to arbitrary EP-indefinite states $\{|\psi^{(i)}\rangle\}$. The subscript SL stands for stochastic LOCC. Then, if this LOCC transformation T_{SL} is executable, there must be full-separable states or biseparable states in the set $\{|\psi^{(i)}\rangle\}$.*

Proof: We prove the present lemma by mathematical induction with respect to N, which is the number of times measurements are performed in the LOCC transformation T_{SL}. Let us define how to count the number of times of the measurement. Let the notation $\mathbb{T}$ stands for an arbitrary LOCC transformation. We fix the order of measurements in the LOCC transformation $\mathbb{T}$ cyclically: If the first measurement of the LOCC transformation $\mathbb{T}$ is performed on the qubit A, the second one is on the qubit B, the third one is on the qubit C, the fourth one returns to the qubit A, and so on. If the first measurement is performed on the qubit B, the second one is on the qubit C, and so on. We can attain such a fixed order by inserting the identity transformation as a measurement. The LOCC transformation $\mathbb{T}$ may have branches and the numbers of times the measurements are performed may be different in different branches. We refer to the largest of the numbers as the number N. We can make the number of each branch equal to N by inserting the identity transformations. An example is given in Fig. B.6. We use this counting procedure in the proofs of other theorems, too.

Let the notations $(C_{AB}, C_{AC}, C_{BC}, \tau_{ABC}, J_5, Q_{\mathrm{e}})$ and $(C_{AB}^{(i)}, C_{AC}^{(i)}, C_{BC}^{(i)}, \tau_{ABC}^{(i)}, J_5^{(i)}, Q_{\mathrm{e}}^{(i)})$ stand for the sets of the C-parameters of the EP-definite state $|\psi\rangle$ and the EP-indefinite states $|\psi^{(i)}\rangle$, respectively.

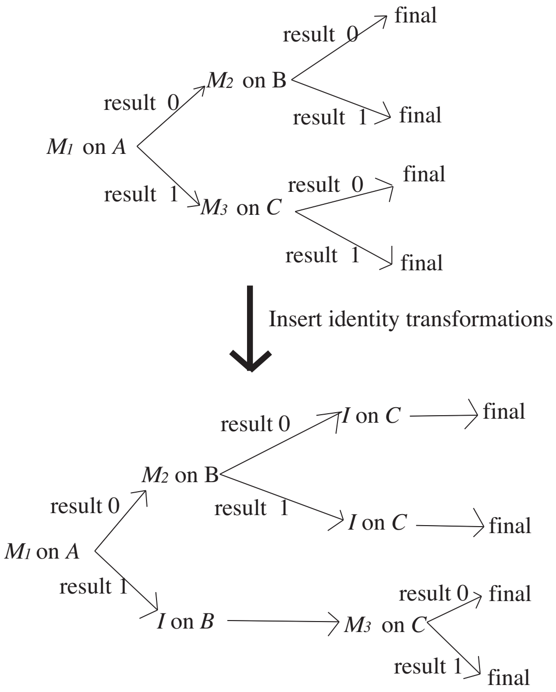

Figure B.6: The method of counting the number N. In this figure, M_1, M_2 and M_3 denote measurements and I denotes the identity transformation. The number N is 3 in this example.

First, we prove the present lemma for $N = 1$. Because of the arbitrariness of the state $|\psi\rangle$, we can assume that the first measurement $\{M_{(i)}|i = 0, 1\}$ of the LOCC transformation T_{SL} is performed on the qubit A without loss of generality. Thus, the operator $M_{(i)}$ makes C_{AB}, C_{AC} and $\sqrt{\tau_{ABC}}$ evenly multiplied by a real number $\alpha^{(i)}$. The state $|\psi\rangle$ is EP definite, and hence C_{AB}, C_{AC} and C_{BC} are all positive. Because the state $\left|\psi^{(i)}\right\rangle$ is EP indefinite, at least one of $C_{AB}^{(i)}$, $C_{AC}^{(i)}$ and $C_{BC}^{(i)}$ has to be zero for all i. When $C_{AB}^{(i)}$ or $C_{AC}^{(i)}$ is zero, the multiplication factor $\alpha^{(i)}$ must be zero, and therefore all of $C_{AB}^{(i)}$, $C_{AC}^{(i)}$ and $\tau_{ABC}^{(i)}$ must be zero. Then, the parameter $J_5^{(i)}$ also must be zero because of $C_{AB}^{(i)} C_{AC}^{(i)} C_{BC}^{(i)} = 0$. Thus, in the case of $C_{AB}^{(i)} = 0$ or $C_{AC}^{(i)} = 0$, the EP-indefinite state $\left|\psi^{(i)}\right\rangle$ is a full-separable state with $C_{BC}^{(i)} = 0$ or a biseparable state with $C_{BC}^{(i)} \neq 0$. Hence, if there were neither a full-separable state nor a biseparable state in the set of EP-indefinite states $\{\left|\psi^{(i)}\right\rangle\}$, the expressions $C_{AC}^{(i)} \neq 0$, $C_{AB}^{(i)} \neq 0$ and $C_{BC}^{(i)} = 0$ would hold for all i. Because of Lemma 17, however, at least one of $C_{BC}^{(0)}$ and $C_{BC}^{(1)}$ would be greater than or equal to C_{BC}, which is positive. This is a contradiction, and thus the expression $C_{BC}^{(i)} \neq 0$ has to hold for at least one of i. We have thereby shown the present lemma for $N = 1$.

Now, we prove Lemma 18 for $N = k + 1$, assuming that Lemma 18 holds whenever $1 \leq N \leq k$. Let us assume that the number of times of measurements in the LOCC transformation T_{SL} from the EP-definite state $|\psi\rangle$ to the EP-indefinite states $\{\left|\psi^{(i)}\right\rangle\}$ is $k + 1$. Because of the assumption for $1 \leq N \leq k$, the situation before the last measurement has to be either of the following two situations:

(i) All states are already EP indefinite, and there are full-separable states or biseparable states among them.

(ii) Some states are EP definite.

In the case of (i), there are full-separable states or biseparable states in the final EP-indefinite states $\{\left|\psi^{(i)}\right\rangle\}$ because an arbitrary full-separable state or an arbitrary biseparable state can be transformed only into full-separable states or biseparable states by a measurement.

In the case of (ii), if there were neither a full-separable state nor a biseparable state in the EP-indefinite states $\{|\psi^{(i)}\rangle\}$, there would have to be a measurement which could transform an EP-definite state to EP-indefinite states which are neither full-separable states nor biseparable states. Because of the theorem for $N = 1$, this is impossible.

Therefore, there must be either full-separable states or biseparable states in the EP-indefinite states $\{|\psi^{(i)}\rangle\}$ in the case (ii) as well as in the case (i). This completes the proof of Lemma 18. □

Because of Lemma 18, if a d-LOCC from an EP-definite state $|\psi\rangle$ to an EP-indefinite state $|\psi'\rangle$ is executable, then $|\psi'\rangle$ is biseparable or full-separable. Without losing generality, we can assume that the only nonzero parameter in the K-parameters of $|\psi'\rangle$ is K'_{BC}. To show the K-parameters of $|\psi\rangle$ and $|\psi'\rangle$ satisfy the condition 1 of Theorem 11, it is sufficient to prove the inequality $K'_{BC} \leq K_{BC}$. To prove $K'_{BC} \leq K_{BC}$, we prove the following Lemma 19.

Lemma 19. *Let the notation $\{M_{(i)}|i = 0, 1\}$ stand for an arbitrary two-choice measurement which is operated on a qubit of a three-qubit pure state $|\psi_{ABC}\rangle$. Note that we can operate $\{M_{(i)}|i = 0, 1\}$ on any one of the qubits A, B and C of the state $|\psi_{ABC}\rangle$. We refer to each result of $\{M_{(i)}|i = 0, 1\}$ as $\left|\psi^{(i)}_{ABC}\right\rangle$. Let the notations ($K_{AB}$,$K_{AC}$,$K_{BC}$,$\tau_{ABC}$,$J_5$,$Q_e$) and ($K^{(i)}_{AB}$,$K^{(i)}_{AC}$,$K^{(i)}_{BC}$,$\tau^{(i)}_{ABC}$,$J^{(i)}_5$,$Q^{(i)}_e$) stand for the sets of the K-parameters of the states $|\psi_{ABC}\rangle$ and $\left|\psi^{(i)}_{ABC}\right\rangle$, respectively. Then, the following inequality holds:*

$$\sum_{i=0}^{1} p_{(i)}\sqrt{K^{(i)}_{BC}} \leq \sqrt{K_{BC}}. \tag{B.88}$$

Proof: First, we prove (B.88) in the case where the measurement $\{M_{(i)}|i = 0, 1\}$ is performed on the qubit B or C. In this case $C^{(i)}_{BC} = \alpha^{(i)}C_{BC}$ and $\sqrt{\tau^{(i)}_{ABC}} = \alpha^{(i)}\sqrt{\tau_{ABC}}$, where $\alpha^{(i)}$ is the multiplication factor of the measurement $\{M_{(i)}|i = 0, 1\}$. Thus, because of (B.79), we can obtain (B.88) as follows:

$$\sum_{i=0}^{1} p_{(i)}\sqrt{K^{(i)}_{BC}} = \sum_{i=0}^{1} p_{(i)}\sqrt{(C^{(i)}_{BC})^2 + \tau^{(i)}_{ABC}} = \sum_{i=0}^{1} p_{(i)}\alpha^{(i)}\sqrt{C^2_{BC} + \tau_{ABC}} \leq \sqrt{K_{BC}}. \tag{B.89}$$

Now, it suffices to prove (B.88) in the case where the first measurement is performed on the qubit A. Let the notation f stand for the left-hand side of (B.88). Because of Lemma 16 we obtain

$$\begin{aligned} f &= \sqrt{b^2C^2_{BC} + 2bk\cos\theta C_{BC}\sqrt{\tau_{ABC}} + ab\tau_{ABC}} \\ &\quad + \sqrt{(1-b)^2C^2_{BC} - 2(1-b)k\cos\theta C_{BC}\sqrt{\tau_{ABC}} + (1-a)(1-b)\tau_{ABC}}, \end{aligned} \tag{B.90}$$

where we substitute θ for the phase $\pi - \theta - \tilde{\varphi}_5$, because the range of the phase θ is from 0 to 2π. When $2k\cos\theta C_{BC} = (b - a)\sqrt{\tau_{ABC}}$, the function f is maximized to $\sqrt{K_{BC}}$. Thus, (B.88) holds. □

The inequality (B.88) includes $K'_{BC} \leq K_{BC}$, if the number N of times measurements of a d-LOCC transformation from $|\psi\rangle$ to $|\psi'\rangle$ is equal to 1. Let us assume that $K'_{BC} \leq K_{BC}$ also holds whenever $1 \leq N \leq k$. Then, when $N = k + 1$, the inequality $K'_{BC} \leq K_{BC}$ also holds; (*Proof*: Let the notion $\{|\psi'^{(i)}\rangle\}$ stand for results of the first measurement the d-LOCC transformation. We refer to the parameter K_{BC} of $|\psi'^{(i)}\rangle$ as $K'^{(i)}_{BC}$. Note that the LOCC transformations from $|\psi'^{(i)}\rangle$ to $|\psi'\rangle$ are d-LOCC transformations whose the number of times measurements are less than or equal to k. Thus, the inequalities $K'_{BC} \leq K'^{(i)}_{BC}$ hold for all of $K'^{(i)}_{BC}$, and thus the inequality $K'_{BC} \leq K_{BC}$ also holds. □) Hence, now we have completed the proof of Theorem 11 in Case $\mathfrak{B}$.

B.3.3 Case $\mathfrak{C}$

In this subsection, we prove Main Theorems in Case $\mathfrak{C}$, where the initial state is EP-indefinite and GHZ-type.

First, we consider the case in which the final state is EP-definite. In this case, the final state is truly multipartite. We cannot achieve a W-type state from a GHZ-type state with an LOCC transformation [67]. Thus, the final state must be a GHZ-type state too. We have already proven that if the initial and final states satisfy the two conditions of Theorem 11, the final state must be GHZ-type. Thus, we only have to consider the case in which both initial and final states are GHZ-type. A d-LOCC transformation from a GHZ-type state whose coefficient set $\{c_i\}$ has a zero to a GHZ-type state whose coefficient set $\{c_i\}$ has no zeros is executable if and only if

$$c'_i \geq c_i \ \ (k = A, B, C), \tag{B.91}$$

$$|z| = 1, \tag{B.92}$$

$$z' \text{ is purely imaginary,} \tag{B.93}$$

where $\{c_i\}$ and z are defined in (B.31) [68]. Because of (B.39), a GHZ-type state is EP-definite if and only if its coefficient set $\{c_i\}$ has no zeros. Thus, in the present case where the final state is EP-definite, we only have to prove that (B.91)–(B.93) are equivalent to the two conditions of Theorem 11.

Let us prove the equivalence between (B.91)–(B.93) are the two conditions of Theorem 11. Because of (B.38) and (B.39), the expressions (B.91)–(B.93) are equivalent to

$$\frac{\tau'_{ABC}}{\tau_{ABC}} \leq \frac{K'_{AB}}{K_{AB}},\ \frac{\tau'_{ABC}}{\tau_{ABC}} \leq \frac{K'_{AC}}{K_{AC}},\ \frac{\tau'_{ABC}}{\tau_{ABC}} \leq \frac{K'_{BC}}{K_{BC}}, \tag{B.94}$$

$$\frac{\sqrt{K_{AB}K_{AC}}}{2\lambda_0^2\sqrt{K_{BC}}} = \frac{\sqrt{K\text{ap}}}{K_5 \pm \sqrt{\Delta_J}} = 1, \tag{B.95}$$

$$\tilde{\varphi}_5 = \pm\frac{\pi}{2}, \tag{B.96}$$

where the double sign $\pm$ in (B.95) is the one in (B.22); note that the possible two sets of $\{\lambda_i, \varphi | i = 0, ..., 1\}$ are $\{\lambda_i^+, \varphi^+ | i = 0, ..., 1\}$ and $\{\lambda_i^-, \tilde{\varphi}^- | i = 0, ..., 1\}$ or $\{\lambda_i^-, \varphi^- | i = 0, ..., 1\}$ and $\{\lambda_i^+, \tilde{\varphi}^+ | i = 0, ..., 1\}$. Because (B.95) is valid in either case of the multiple signs, the parameter Δ_J is zero. Because of $\Delta_J = K_5^2 - K\text{ap}$, when $\Delta_J = 0$ holds, (B.95) also holds. Thus, (B.95) is equivalent to $\Delta_J = 0$. Because of $\sqrt{J\text{ap}}\cos\tilde{\varphi}_5 = J_5$, (B.96) is equivalent to $J_5 = J\text{ap} = 0$. Thus, (B.95) and (B.96) are equivalent to (B.14). We have already proven that (B.14) is equivalent to $\zeta_{\text{lower}} \leq \zeta \leq 1$ and (B.17) in the section B.3.1. Thus, we only have to prove that (B.94) is equivalent to the existence of ζ, $0 \leq \zeta_A \leq 1$, $0 \leq \zeta_B \leq 1$ and $0 \leq \zeta_C \leq 1$, which satisfy (B.12). We can define such ζ–ζ_C as (B.45) and (B.46). Thus, in the case where the final state is EP-definite, the conditions of Theorem 11 is a necessary and sufficient condition of d-LOCC.

Second, we consider the case where the final state is EP-indefinite and GHZ-type. Because a GHZ-type state is EP-definite if and only if its coefficient set $\{c_i\}$ has no zeros, in this case, a d-LOCC transformation is executable if and only if

$$c_i' \geq c_i \ \ (k = A, B, C), \tag{B.97}$$

$$|z'| \geq |z|, \tag{B.98}$$

where $\{c_i\}$ and z are defined in (B.31), and where we choose z and z' such that $|z| \geq 1$ and $|z'| \geq 1$ [68].

Let us prove that (B.97) and (B.98) are equivalent to the condition 1 of Theroem 2. Because of (B.22), (B.38), $|z'| \geq 1$ and $|z| \geq 1$,

$$|z| = \frac{\sqrt{K_{\mathrm{ap}}}}{K_5 - \sqrt{\Delta_J}}, \ \ |z'| = \frac{\sqrt{K'_{\mathrm{ap}}}}{K'_5 - \sqrt{\Delta'_J}}. \tag{B.99}$$

Because of (B.39), (B.97) is equivalent (B.94). Because both of the initial and final states are EP-indefinite, $J_5 = J_5' = 0$ is valid. Thus, we can define $\zeta_{\mathrm{lower}} \leq \zeta \leq 1$, $0 \leq \zeta_A \leq 1$, $0 \leq \zeta_B \leq 1$ and $0 \leq \zeta_C \leq 1$, which satisfy (B.12) as (B.45) and (B.46). Thus, in the case where the final state is EP-indefinite and GHZ-type, the conditions of Theorem 11 is a necessary and sufficient condition of d-LOCC.

Third, we consider the case where the final state is EP-indefinite but not GHZ-type. In this case, the final state is biseparable or full-separable. Because the final state is not EP-definite, the condition 2 of Theorem 11 is left out; we only have to consider the condition 1. When the final state is full-separable, a d-LOCC transformation to the final state is clearly executable, and the initial and final states clearly satisfy the condition 1 of Theorem 11: $\zeta_A = \zeta_B = \zeta_C = 0$ satisfy (B.12). Thus, we only have to consider the case the final state is biseparable.

Let us prove the condition 1 of Theorem 11 is a necessary condition of the possibility of the d-LOCC transformation. Without loss of generality, we can assume that the only nonzero K-parameter of the final state is K'_{BC}. Because of Lemma 19, we can prove the inequality $K'_{BC} \leq K_{BC}$, in the same manner as $K'_{BC} \leq K_{BC}$ is shown in Case $\mathfrak{B}$. Thus, if a d-LOCC transformation is executable, the initial and final states satisfy the condition 1 of Theorem 11. In other words, the condition 1 of Theorem 11 is a necessary condition of the possibility of the d-LOCC transformation.

Finally, let us prove the condition 1 of Theorem 11 is a sufficient condition of the possibility of the d-LOCC transformation. Without loss of generality, we can assume that the only nonzero K-parameter of the final state is K'_{BC}. The upper limit of K'_{BC} is K_{BC}. We can realize this upper limit by the measurement $\{M_{(i)}\}$ which is defined as (B.82)–(B.87). According to Ref. [69], the set of full-separable states and biseparable states which have the same kind of bipartite entanglement is a totally ordered set. Thus, in this case, a d-LOCC transformation from $|\psi\rangle$ to $|\psi'\rangle$ is executable if and only if $K'_{BC} \leq K_{BC}$. Thus, in the case where the final state is EP-indefinite and not GHZ-type, the conditions of Theorem 11 is a necessary and sufficient condition of the possibility of d-LOCC transformation. □

B.3.4 Case $\mathfrak{D}$

In this subsection, we prove Theorem 10 in Case $\mathfrak{D}$, where the tangle of the initial state is zero.

First, we simplify (B.12). Let us show that we can leave τ_{ABC}, J_5 and Q_{e} out of the discussion hereafter. First, $\tau'_{ABC} = 0$ follows from $\tau_{ABC} = 0$, because an arbitrary measurement makes the tangle τ_{ABC} only multiplied by a constant. Next, because of (B.2)–(B.4) and the equation $\tau_{ABC} = 0$, the equation $J_5 = C_{AB}C_{AC}C_{BC}$ holds. (*Proof*: Because of (B.3) and $\tau_{ABC} = 0$, at least one of λ_0 and λ_4 is zero. When λ_0 is zero, the equations $J_5 = C_{AB}C_{AC}C_{BC} = 0$ hold. Thus λ_4 is zero, and then $J_5 = C_{AB}C_{AC}C_{BC} = 4\lambda_0^2\lambda_2^2\lambda_3^2$ follows (B.2) and (B.4).□) Thus, in order to examine the change of J_5, it suffices to examine the change of the concurrences C_{AB}, C_{AC} and C_{BC}.

Next, because of $\tau_{ABC} = 0 \Leftrightarrow \lambda_0 = 0 \vee \lambda_4 = 0$ and because if there is a zero in $\{\lambda_k | k = 0, ..., 4\}$ then $\sin\varphi = 0$, the equation $Q_\mathrm{e} = 0$ follows (B.6). In the same manner, the entanglement charge Q'_e is also zero because of $\tau'_{ABC} = 0$. Thus, $Q_\mathrm{e} = Q'_\mathrm{e} = 0$ holds. Condition 2 of Theorem 11 satisfies this equation. Let us show this. The state $|\psi\rangle$ is $\tilde{\zeta}$-indefinite, because $\tau_{ABC} = 0$:

$$\begin{aligned}\Delta_J = K_5^2 - K_\mathrm{ap} = J_5^2 - J_\mathrm{ap} = C_{AB}^2 C_{AC}^2 C_{BC}^2 \sin^2\varphi_5 \\ = 4C_{AB}^2 C_{AC}^2 \lambda_1^2 \lambda_4^2 \sin^2\varphi = 0,\end{aligned} \tag{B.100}$$

where we use $\sin\varphi = 0$. Note that $\sin\varphi = 0$ holds when there is a zero in $\{\lambda_i | i = 0, ..., 4\}$ and that $\tau_{ABC} = \lambda_0\lambda_4 = 0$. Because the state $|\psi\rangle$ is $\tilde{\zeta}$-indefinite, Condition 2 is reduced to $|Q'_\mathrm{e}| = \mathrm{sgn}[(1-\zeta)(\zeta - \zeta_\mathrm{lower})]$. Incidentally, because of $\tau_{ABC} = 0$, $\zeta_\mathrm{lower} = 1$ holds. Thus, $\zeta = 1$ follows $\zeta_\mathrm{lower} \le \zeta \le 1$, and thus Condition 2 satisfies the equation $Q'_\mathrm{e} = 0$. In order to prove the present theorem, it suffices to show that a necessary and sufficient condition is that there are real numbers α_A, α_B and α_C which are from zero to one and which satisfy the following equation:

$$\begin{pmatrix} C'^2_{AB} \\ C'^2_{AC} \\ C'^2_{BC} \end{pmatrix} = \begin{pmatrix} \alpha_A^2\alpha_B^2 & & \\ & \alpha_A^2\alpha_C^2 & \\ & & \alpha_B^2\alpha_C^2 \end{pmatrix} \begin{pmatrix} C^2_{AB} \\ C^2_{AC} \\ C^2_{BC} \end{pmatrix}. \tag{B.101}$$

Note that (B.101), $J_5 = C_{AB}C_{AC}C_{BC}$ and $J'_5 = C'_{AB}C'_{AC}C'_{BC}$ give $J'_5 = \alpha_A^2\alpha_B^2\alpha_C^2 J_5$, and that $\tau_{ABC} = 0 \Rightarrow (K_{AB} = C_{AB}^2) \wedge (K_{AC} = C_{AC}^2) \wedge (K_{BC} = C_{BC}^2)$.

We can classify the sets of the initial and final states as follows:

Case $\mathfrak{D}$-1: At least one of the concurrences C_{AB}, C_{BC} and C_{AC} is zero.

Case $\mathfrak{D}$-2: None of the concurrences C_{AB}, C_{BC} and C_{AC} is zero, and at least one of the concurrences C'_{AB}, C'_{BC} and C'_{AC} is zero.

Case $\mathfrak{D}$-3: All of the concurrences C_{AB}, C_{BC}, C_{AC}, C'_{AB}, C'_{BC} and C'_{AC} are nonzero.

Note that we already have $\tau_{ABC} = \tau'_{ABC}$ in the present Case $\mathfrak{D}$.

In Case $\mathfrak{D}$-1, we first note that only the biseparable states are allowed as the initial states in this case. The set of full-separable states and biseparable states which have the same kinds of bipartite entanglements is a totally ordered set [69]. We cannot transform a full-separable state or a biseparable state into other type states with LOCC transformations [67], and thus we can derive the necessary and sufficient condition, which reduces to the following: there is an executable deterministic LOCC transformation from $|\psi\rangle$ to $|\psi'\rangle$ if and only if $C_{AC} \ge C'_{AC}$. This condition is equivalent to (B.101) in Case $\mathfrak{D}$-1.

In Case $\mathfrak{D}$-2, where none of C_{AB}, C_{BC} and C_{AC} is zero and at least one of C'_{AB}, C'_{BC} and C'_{AC} is zero, the initial state is EP definite while the final state is EP indefinite. Thus, Case $\mathfrak{B}$ includes Case $\mathfrak{D}$-2, and thus the existence of α_A, α_B and α_C which satisfy (B.101) is the necessary and sufficient condition.

In Case $\mathfrak{D}$-3, where all of the concurrences C_{AB}, C_{BC}, C_{AC}, C'_{AB}, C'_{BC} and C'_{AC} are nonzero, the initial and final states are W-type states. In the present case, we can use the result of Ref. [70]. A d-LOCC transformation from a W-type state $|\psi\rangle$ to another W-type state $|\psi'\rangle$ is possible if and only if

$$x_i \geq x_i' \ \ (i = 1, 2, 3), \tag{B.102}$$

where the sets of positive real numbers $\{x_i\}$ and $\{x_i'\}$ are defined by the decompositions of $|\psi\rangle$ and $|\psi'\rangle$ [70]:

$$|\psi\rangle = x_0 |000\rangle + x_1 |100\rangle + x_2 |010\rangle + x_3 |001\rangle\,, \tag{B.103}$$

$$|\psi'\rangle = x_0' |000\rangle + x_1' |100\rangle + x_2' |010\rangle + x_3' |001\rangle\,. \tag{B.104}$$

Note that we can reduce (B.103) into a generalized Schmidt decomposition

$$|\psi\rangle = x_1 |000\rangle + x_0 |100\rangle + x_3 |101\rangle + x_2 |110\rangle \tag{B.105}$$

with transformation $|0_A\rangle \leftrightarrow |1_A\rangle$. We thereby obtain

$$2x_1x_2 = C_{AB}, \ \ 2x_1x_3 = C_{AC}, \ \ 2x_2x_3 = C_{BC}, \tag{B.106}$$

$$x_1 = \sqrt{\frac{C_{AB}C_{AC}}{2C_{BC}}}, \ \ x_2 = \sqrt{\frac{C_{AB}C_{BC}}{2C_{AC}}}, \ \ x_1 = \sqrt{\frac{C_{AC}C_{BC}}{2C_{AB}}}. \tag{B.107}$$

Thus, the existence of α_A, α_B and α_C which are from zero to one which satisfy (B.101) is equivalent to the existence α_A, α_B and α_C which are from zero to one which satisfy

$$\alpha_A = x_1'/x_1, \ \ \alpha_B = x_2'/x_2, \ \ \alpha_C = x_3'/x_3. \tag{B.108}$$

Note that when α_A, α_B and α_C are from 0 to 1, (B.108) is equivalent to (B.102). Thus, (B.101) is a necessary and sufficient condition of d-LOCC in Case $\mathfrak{D}$-3. □

We thereby have completed the proof of Theorem 11 in all cases.

Appendix C

Thermodynamical derivation of (4.7)

In the present appendix, we derive the inequality (4.7) in the thermodynamical way. Hereafter, we treat the working body S, and the hot heat bath B_H, and the cold heat bath B_L as the finite-size thermodynamic systems. We express the equiliburium states of S, B_H and B_L as (U_S, X_S), (U_{B_H}, X_{B_H}) and (U_{B_L}, X_{B_L}), where U is the internal energy and X is the set of other thermodynamic variables. Initially, the systems S, B_H and B_L are in the equilibrium states $(U_S^{\mathrm{ini}}, X_S^{\mathrm{ini}})$, $(U_{B_H}^{\mathrm{ini}}, X_{B_H}^{\mathrm{ini}})$ and $(U_{B_L}^{\mathrm{ini}}, X_{B_L}^{\mathrm{ini}})$, respectively. Then, we perform an adiabatic operation on the three systems. During the adiabatic operation, the hot bath B_H loses the heat Q_H, and we take the extracted work W_{ext}. After the adiabatic operation, we wait enough time, and these three systems are assumed to be in equilibrium states $(U_S^{\mathrm{ini}}, X_S^{\mathrm{ini}})$, $(U_{B_H}^{\mathrm{ini}} - Q_H, X_{B_H}^{\mathrm{ini}})$, and $(U_{B_L}^{\mathrm{ini}} + Q_H - W_{\mathrm{ext}}, X_{B_L}^{\mathrm{ini}})$.

Under the above setup, let us derive an upper bound for the efficiency. Because the adiabatic transformation does not decreases the thermodynamic entropy,

$$S(U_S^{\mathrm{ini}}, X_S^{\mathrm{ini}}) + S(U_{B_H}^{\mathrm{ini}}, X_{B_H}^{\mathrm{ini}}) + S(U_{B_L}^{\mathrm{ini}}, X_{B_L}^{\mathrm{ini}}) \leq S(U_S^{\mathrm{ini}}, X_S^{\mathrm{ini}}) + S(U_{B_H}^{\mathrm{ini}} - Q_H, X_{B_H}^{\mathrm{ini}}) + S(U_{B_L}^{\mathrm{ini}} + Q_H - W_{\mathrm{ext}}, X_{B_L}^{\mathrm{ini}}) \tag{C.1}$$

holds. Because the thermodynamic entropy is an increasing function of the internal energy, we obtain

$$W_{\mathrm{ext}} \leq Q_H + U_{B_L}^{\mathrm{ini}} - U'_{B_L} \tag{C.2}$$

where U'_{B_L} is defined by $S(U_{B_H}^{\mathrm{ini}}, X_{B_H}^{\mathrm{ini}}) + S(U_{B_L}^{\mathrm{ini}}, X_{B_L}^{\mathrm{ini}}) = S(U_{B_H}^{\mathrm{ini}} - Q_H, X_{B_H}^{\mathrm{ini}}) + S(U'_{B_L}, X_{B_L}^{\mathrm{ini}})$. Thus,

$$\eta := \frac{W_{\mathrm{ext}}}{Q_H} = 1 - \frac{U'_{B_L} - U_{B_L}^{\mathrm{ini}}}{Q_H}. \tag{C.3}$$

The (C.3) is equivalent to (4.7). □

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