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Quantum Thermodynamics with Measurement Processes
（測定過程のある量子熱力学）

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Department of Physics, Graduate School of Science,
The University of Tokyo
東京大学大学院理学系研究科物理学専攻

Yohei Morikuni
森國　洋平

Abstract

Quantum thermodynamics is thermodynamics extended to be applied to microscope quantum systems. The conventional studies of quantum thermodynamics are based on two assumptions: first, the dynamics of the microscope quantum system is described by the unitary evolution; second, the work performed on an external agent is equal to the energy loss of the microscope quantum system. However, several studies pointed out that these assumptions are not compatible with each other.

As an alternative to the conventional approach, it has been proposed to describe the dynamics of the microscope quantum system as a quantum measurement process. This proposition made based on the analogy between the work extraction of thermodynamics and the measurement process of quantum mechanics, implying that quantum thermodynamics is essentially quantum-measurement theory.

In the present thesis, we first derive a quantum version of the Jarzynski equality using the new approach. Our derivation correctly contains information about the fluctuation of the actual work, namely, the energy gain of the external agent. Our derivation enables us to analyze the influence of the quantum measurement quantitatively.

Our derivation of the Jarzynski equality describes the fluctuation of the actual work under the actual dynamics, but is unclear how the microscopic quantum system is operated by the external agent. To resolve this issue, we next consider the continuous measurement of the control parameter and derive the quantum Jarzynski equality under the continuously monitoring control parameter. We can thereby obtain the relation between the control parameter and the second law of thermodynamics.

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Chapter 1

Introduction

Thermodynamics is one of the fundamental and important theories in physics [4]. It characterizes to macroscopic systems in terms of several macroscopic physical quantities without resorting to microscopic details of the macroscopic systems. In other words, thermodynamics is a universal theory on macroscopic systems.

The most important characteristic of thermodynamics is the irreversibility of the macroscopic systems. This irreversibility is a unique property not found in other fundamental theories of physics and is known as the second law of thermodynamics. The second law of thermodynamics, yields limitations of dynamics of the macroscopic systems; for example, an upper bound of the work performed by the macroscopic system and one of the efficiency of macroscopic heat engines [1], which are transducers of the heat to the work.

Since the macroscopic system consists of a huge number of microscopic degrees of freedom, it is one of the major issues in physics to derive thermodynamics from microscopic mechanics. One answer is statistical mechanics [10], which is a theory that associates the statistical properties of microscopic degrees of freedom with the thermodynamics of quantities, and thus describes the equilibrium of the macroscopic systems.

A new demand arises because the recent development of experimental technology lets us observe and operate microscopic systems; we can perform experiments of molecular motors in cells [21], a box containing a single electron [90] and so on [33, 59, 65, 72, 97, 98]. Because these experiments are performed on microscopic systems, we cannot directly apply thermodynamics to them. Accordingly, many researchers have been trying to extend thermodynamics in order to apply it to microscopic systems.

Quantum thermodynamics is thermodynamics extended to be applied to microscopic quantum systems [116]. It utilizes a combination of statistical and quantum mechanics, adopting a model of a microscopic quantum system connected to an external agent. Many conventional studies [8, 9, 23, 25, 27, 30, 32, 36, 39, 40, 42, 46, 48, 50, 52, 54, 68, 70, 71, 73, 79, 80, 85, 88, 94, 95, 103, 116] of quantum thermodynamics use two assumptions: first, the dynamics of the microscopic quantum system is described by the unitary evolution generated by a time-dependent Hamiltonian of the microscopic quantum system; second, the work performed on the external agent is equal to the energy loss of the microscopic quantum system. In this conventional approach, we can derive not only the second law of thermodynamics [7, 9, 26, 43, 56, 57, 63, 69, 85, 89, 105, 115] but also many results such as the fluctuation theorem [23, 25, 30, 40, 48], which describes the fluctuation of physical quantities in microscopic systems, and information thermodynamics [46, 50, 54, 70, 71, 73, 79, 80, 88, 94, 95, 103], which is thermodynamics with feedback processes taken into account.

The conventional approach indeed gives some properties of thermodynamics. However, several studies [93, 114, 117, 119, 122] pointed out that the two assumptions above are not compatible with each other. For example, if the actual dynamics of the microscopic quantum system is approximated to the unitary evolution, the statistical properties of the energy loss of the microscopic quantum system and the energy obtained by the external agent behave differently. Therefore, the assumptions of the conventional approach is inappropriate to quantum thermodynamics. Accordingly, we needs to find a different approach to study quantum thermodynamics.

As an alternative to the conventional approach, is has been proposed to describe the dynamics of the microscopic quantum system as a quantum measurement process [93, 117, 120]. This proposition was made based on the analogy between the work extraction in thermodynamics and the quantum measurement process. The work extraction is a process in which an external agent operates a system and obtains quantities of the work. On the other hand, the measurement is a process in which an external agent operates a system to observe and obtains physical quantities. This approach implies that quantum thermodynamics is essentially quantum-measurement theory. Therefore, we need to take into account the influence of measurements in thermodynamics.

In the present thesis, we study quantum thermodynamics using the new approach, which describes the work extraction processes as measurement processes. First, we consider the Jarzynski equality, which describes a statistical property of the extracted work, under the new approach to research the influence of the quantum measurement. Our derivation of the Jarzynski equality correctly contains information about the fluctuation of the actual work, namely, the energy gain of the external agent, and is essentially different from the conventional derivation of one [23, 25, 30, 40, 48]. The influence of the measurement appears in the Jarzynski equality as the difference of a constant and the constant is determined by the measurement process.

Our derivation of the Jarzynski equality describes the fluctuation of the actual work under the actual dynamics. However, it is unclear as to how the microscopic quantum system is operated by the external agent. To resolve this issue, we next consider the continuous measurement of the control parameter, which describes the operation by the external agent. By combining the now approach of the work extraction and the formulation of the continuous measurement, we obtain the parameter-dependent Jarzynski equality as well as the relation between the control parameter and the second law of thermodynamics.

The present thesis is organized as follows. In the chapter 2, we describe the general theory of quantum dynamics and measurement. In the chapter 3, we review the conventional approach of quantum thermodynamics and the derived results. This chapter has the three sections about the definition of the conventional approach, the second law of thermodynamics and the fluctuation theorems. In the chapter 4, we explain the problem of the conventional approach of quantum thermodynamics and review the new approach describing the work extraction of thermodynamics as the measurement process of quantum mechanics [93, 117]. In the chapter 5, we derive a quantum version of the Jarzynski equality based on the new approach of the chapter 4. The results in the chapter 5 are based on the references [119] under the author's collaboration with Dr. H. Tajima and Prof. N. Hatano. In the chapter 6, we derive a quantum version of the Jarzynski equality under continuously monitored control parameter. The section 6.1.1 in the chapter 6 is a short review of the time reversal introduced in the reference [121]. The other sections in the chapter 6 is the results of the author under the collaboration with Dr. H. Tajima.

Chapter 2

Quantum dynamics and measurement

2.1 Quantum dynamics

In this section, we first describe a unitary evolution, which is a fundamental time evolution in quantum mechanics and is applicable to a closed quantum system. Next, we introduce a general quantum dynamics, which can be applied both to a open and closed quantum systems.

2.1.1 Unitary evolution

Let us consider a closed quantum system. In quantum mechanics, the state of an isolated quantum system is represented by a unit vector $|\psi\rangle$, whose time evolution follows the Schrödinger equation

$$i\hbar\frac{d}{dt}\left|\psi(t)\right\rangle = H(t)\left|\psi(t)\right\rangle, \tag{2.1}$$

where $H(t)$ is the generally time-dependent Hamiltonian of the system.

The time evolution

$$|\psi(t)\rangle = U(t,t_0)\,|\psi(t_0)\rangle \tag{2.2}$$

defined the unitary operator $U(t,t_0)$, which is satisfies $U(t_0,t_0)=I$ with identity operator I. Inserting the equation (2.2) into the Schrödinger equation (2.1), we obtain

$$i\hbar\frac{d}{dt}U(t,t_0) = H(t)U(t,t_0); \tag{2.3}$$

in other words, the operator $U(t,t_0)$ satisfies the Schrödinger equation. Therefore, the operator $U(t,t_0)$ is given by

$$U(t,t_0) = \mathbb{T}\exp\left[-\frac{i}{\hbar}\int_{t_0}^{t} ds\,H(s)\right], \tag{2.4}$$

where $\mathbb{T}$ is time ordering. From the equation (2.4), we obtain

$$U(t_2,t_0) = U(t_2,t_1)U(t_1,t_0), \tag{2.5}$$

$$U^\dagger(t_1,t_0) = U(t_0,t_1) \tag{2.6}$$

for $t_0 \leq t_1 \leq t_2$.

In the above description, the state of the system is represented by a unit vector and is called a pure state. We can extend the state of the system to statistical mixture of pure states, which is called a mixed state. The mixed state is described by a Hermitian operator ρ, which is called the density matrix. For the mixture of pure states $|\Psi_i\rangle$ and the corresponding probability p_i satisfying $\sum_i p_i = 1$, the density matrix ρ is given by

$$\rho = \sum_i p_i |\Psi_j\rangle\langle\Psi_j|. \tag{2.7}$$

Using the Schrödinger equation (2.1) in the time derivative of the density matrix (2.7), we obtain

$$i\hbar\frac{\partial\rho(t)}{\partial t} = [H(t), \rho(t)] \tag{2.8}$$

with $[A, B] \coloneqq AB - BA$. This is called the von Neumann equation. Similarly to the pure state, the time evolution of the density matrix is given by the unitary operator $U(t, t_0)$ of the equation (2.4) in the form

$$\rho(t) = U(t, t_0)\rho(t_0)U^\dagger(t, t_0). \tag{2.9}$$

2.1.2 General quantum dynamics

In the previous section, we showed that the time evolution of the closed quantum system is represented by a unitary operator. However, in the case of an open quantum system, we cannot generally represent the time evolution in terms of a unitary operator.

To consider the time evolution of the open quantum system, we introduce an environment interacting with the system of interest and trace it out after the time evolution.

We assume that the composition of the system S of interest and the environment E is a closed quantum system. Hence, the composite system is evolved under a unitary operator U of the composite system. Let ρ and σ_E denote the initial states of the system S and the environment E, respectively. Then, the time evolution of the system S is given by a map $\mathcal{K}$ in the form

$$\mathcal{K}(\rho) \coloneqq \mathrm{Tr}_\mathrm{E}\big[U(\rho \otimes \sigma_\mathrm{E})U^\dagger\big], \tag{2.10}$$

where Tr_E denotes the partial trace over the environment E. This map $\mathcal{K}$ describes the general time evolution of the system S of interest and is called a quantum channel or quantum operation in quantum information theory [24, 108]. Of course, the unitary evolution in the section 2.1.1 is a simple case of the quantum channel. From the equation (2.9), the map $\mathcal{U}_{t,t_0}$ of the unitary evolution is given by

$$\mathcal{U}_{t,t_0}(\rho) = U(t, t_0)\rho U^\dagger(t, t_0). \tag{2.11}$$

The time-evolution map $\mathcal{K}$ of the equation (2.10) has the following properties:

Affine property (convex linear) For any density matrices ρ_1 and ρ_2 and for a real number $p \in [0, 1]$, there satisfies

$$\mathcal{K}(p\rho_1 + (1-p)\rho_2) = p\mathcal{K}(\rho_1) + (1-p)\mathcal{K}(\rho_2). \tag{2.12}$$

Trace preserving For any density matrix ρ, there satisfies $\mathrm{Tr}(\mathcal{K}(\rho)) = \mathrm{Tr}(\rho)$.

Completely Positive For any positive operator A_S on the system S, $\mathcal{K}(A_\mathrm{S})$ is also the positive operator. Moreover, if we introduce an extra system R of arbitrary dimension, $(\mathcal{K} \otimes \mathcal{I}_\mathrm{R})(A_\mathrm{SR})$ is the positive operator for any positive operator A_SR on the composite system SR, where $\mathcal{I}_\mathrm{R}$ denotes the identity map on the extra system R.

We can show the three properties of time-evolution map from the equation (2.10); in other words, the time-evolution map is a trace-preserving completely positive (TPCP) map [108]. Conversely, we can drive the equation (2.10) from any map $\mathcal{K}$ that satisfies the three properties of TPCP map. Therefore, the TPCP map can always represent the environment model of the equation (2.10) [24, 108].

The time-evolution map (2.10) has another representation known as the Kraus representation [108] and the operator-sum one [24]. The Kraus representation of the TPCP map is given by the following: for a TPCP map $\mathcal{K}$, there exists a set of linear operators $\{ K_n \}_n$ satisfying $\sum_n K_n^\dagger K_n = I$, where I is the identity operator, such that

$$\mathcal{K}(\rho) = \sum_n K_n \rho K_n^\dagger \tag{2.13}$$

for an arbitrary operator ρ. The operator K_n in the equation (2.13) is called the Kraus operator.

Let us derive the Kraus operator explicitly. Assume the eigenvalue decomposition of the initial state σ_E in the equation (2.10) in the form

$$\sigma_\mathrm{E} = \sum_i q_i |\psi_i\rangle_\mathrm{E}\langle\psi_i| \tag{2.14}$$

with $\sum_i q_i = 1$ and ${}_\mathrm{E}\big\langle\psi_i \,\big|\, \psi_j\big\rangle_\mathrm{E} = \delta_{i,j}$. The equation (2.10) thereby becomes

$$\mathcal{K}(\rho) = \sum_{i,j} \tilde{K}_{i,j} \rho \tilde{K}_{i,j}^\dagger \tag{2.15}$$

with $\tilde{K}_{i,j} \coloneqq \sqrt{q_i}\, {}_\mathrm{E}\big\langle\psi_j \,\big|\, U \,\big|\, \psi_i\big\rangle_\mathrm{E}$. Because the operator $\tilde{K}_{i,j}$ satisfies

$$\begin{aligned} \sum_{i,j} \tilde{K}_{i,j}^\dagger \tilde{K}_{i,j} &= \sum_{i,j} q_i \mathrm{Tr}_\mathrm{E}\Big[|\psi_i\rangle_\mathrm{E}\langle\psi_i| U^\dagger |\psi_j\big\rangle_\mathrm{E}\big\langle\psi_j| U\Big] & (2.16) \\ &= \mathrm{Tr}_\mathrm{E}[I \otimes \sigma_\mathrm{E}] = I, & (2.17) \end{aligned}$$

the set of the operators $\{ \tilde{K}_{i,j} \}_{i,j}$ is a set of the Kraus operators of the time-evolution map $\mathcal{K}$. Thus, we can obtain a Kraus representation from the equation (2.10).

2.2 Quantum measurement

In this section, we describe measurement theory of quantum systems. We first introduce the projection measurement and secondly the general quantum measurement. Finally, we show a continuous measurement as a limitation of a series of repeated measurements.

2.2.1 Projection measurement

The projection measurement is a fundamental measurement in quantum mechanics. Let us consider the projection measurement of a physical quantity A. The physical quantity A is denoted by a Hermitian operator and has the spectral decomposition

$$A = \sum_a a P_a, \tag{2.18}$$

where a and P_a denote the eigenvalue of the observable A and the corresponding projection, respectively. Given a state ρ of a system, the probability that the outcome of the measurement is the eigenvalue a is given by

$$\Pr(A = a|\rho) \coloneqq \mathrm{Tr}[P_a \rho], \tag{2.19}$$

which is called the Born rule [108]. Of course, the summation of the probability $\Pr(A = a|\rho)$ with respect to the outcome a is equal to unity, because the projection P_a satisfies $\sum_a P_a = I$ with the identity operator I.

In general, the state changes after the measurement. When we obtain an outcome a by the projection measurement, the post-measurement state depends on the outcome a, given by

$$\rho_a \coloneqq \frac{P_a \rho P_a}{\Pr(A = a|\rho)}. \tag{2.20}$$

On the other hand, when we perform the projection measurement but do not know the measurement outcome, the post-measurement state becomes the statistical mixture of the equation (2.20) of each outcome, given by

$$\rho' \coloneqq \sum_a \Pr(A = a|\rho)\rho_a = \sum_a P_a \rho P_a. \tag{2.21}$$

The situations of the equations (2.20) and (2.21) are called selective measurement and non-selective measurement, respectively [108].

In particular, when P_a projects states onto the normalized eigenstate $|\phi_a\rangle$ of the eigenvalue a, namely $P_a = |\phi_a\rangle\langle\phi_a|$, the probability (2.19) is given by $\Pr(A = a|\rho) = \langle\phi_a \,|\, \rho \,|\, \phi_a\rangle$ and the corresponding selective measurement (2.20) becomes the pure state of the eigenstate $|\phi_a\rangle$:

$$\rho_a = \frac{|\phi_a\rangle\langle\phi_a|\rho|\phi_a\rangle\langle\phi_a|}{\langle\phi_a \,|\, \rho \,|\, \phi_a\rangle} = |\phi_a\rangle\langle\phi_a|. \tag{2.22}$$

2.2.2 General quantum measurement

To consider a general quantum measurement, we can use an indirect measurement model, which is described by the time evolution of a system composed by a system of interest and a measurement device. The measurement device interacts with the system of interest and extracts information out of it. After the interaction, we observe the measurement device and indirectly obtain the information of the system of interest from the measurement device.

Let us assume that the system composed by the system S of interest and the measurement device D is a closed quantum system. Let ρ and σ_{D} denote an arbitrary initial state of the system S and an initial state of the measurement device D, respectively. The initial state of the composite system is given by $\rho \otimes \sigma_{\mathrm{D}}$. Since the composite system is a closed quantum system, it evolve accordingly to a unitary operator U into the state $U(\rho \otimes \sigma_{\mathrm{D}})U^{\dagger}$. After the time evolution, we measure a physical quantity A_{D} of the measurement device D, which is called a meter observable. The spectral decomposition of A_{D} is given by

$$A_{\mathrm{D}} = \sum_{a} a P_{a}^{\mathrm{D}} \tag{2.23}$$

where a and P_{a}^{D} denote the eigenvalue of A_{D} and the corresponding projection, respectively.

Suppose that we obtain an outcome a after the measurement of the meter observable, which is the selective measurement of the composite system. The post-measurement state (2.20) for the outcome a is given by

$$\rho_{a}^{\mathrm{SD}} := \frac{\left(I_{\mathrm{S}} \otimes P_{a}^{\mathrm{D}}\right) U(\rho \otimes \sigma_{\mathrm{D}}) U^{\dagger} \left(I_{\mathrm{S}} \otimes P_{a}^{\mathrm{D}}\right)}{\Pr\left(A_{\mathrm{D}} = a \middle| U(\rho \otimes \sigma_{\mathrm{D}}) U^{\dagger}\right)}, \tag{2.24}$$

where I_{S} is the identity operator on S. Note that we replaced P_{a} in the equation (2.20) with $I_{\mathrm{S}} \otimes P_{a}^{\mathrm{D}}$ because the measurement of the meter observable is not supposed to affect the system S. The denominator $\Pr\left(A_{\mathrm{D}} = a \middle| U(\rho \otimes \sigma_{\mathrm{D}}) U^{\dagger}\right)$ is the probability of the specific outcome a given the state $U(\rho \otimes \sigma_{\mathrm{D}})U^{\dagger}$ of the system S in the form

$$\Pr\left(A_{\mathrm{D}} = a \middle| U(\rho \otimes \sigma_{\mathrm{D}}) U^{\dagger}\right) := \mathrm{Tr}\left[\left(I_{\mathrm{S}} \otimes P_{a}^{\mathrm{D}}\right) U(\rho \otimes \sigma_{\mathrm{D}}) U^{\dagger}\right]. \tag{2.25}$$

We now focus on the measurement of the system S of interest. Tracing the equation (2.24) over the measurement device D, we obtain the post-measurement state of the system S depending on the outcome a in the from

$$\rho_{a}^{\mathrm{S}} := \mathrm{Tr}_{\mathrm{D}}\left[\rho_{a}^{\mathrm{SD}}\right] = \frac{\mathcal{M}_{a}(\rho)}{\Pr\left(A_{\mathrm{D}} = a \middle| U(\rho \otimes \sigma_{\mathrm{D}}) U^{\dagger}\right)}, \tag{2.26}$$

where Tr_{D} is partial trace over the measurement device D and a map $\mathcal{M}_{a}$ depending on the outcome a as

$$\mathcal{M}_{a}(\rho) := \mathrm{Tr}_{\mathrm{D}}\left[\left(I_{\mathrm{S}} \otimes P_{a}^{\mathrm{D}}\right) U(\rho \otimes \sigma_{\mathrm{D}}) U^{\dagger} \left(I_{\mathrm{S}} \otimes P_{a}^{\mathrm{D}}\right)\right]. \tag{2.27}$$

The probability (2.25) is written as

$$\Pr\left(A_{\mathrm{D}} = a \middle| U(\rho \otimes \sigma_{\mathrm{D}}) U^{\dagger}\right) = \mathrm{Tr}[\mathcal{M}_{a}(\rho)]. \tag{2.28}$$

Because the right hand side of the above probability depends on the initial state ρ and the outcome a, we can rewrite the equations (2.26) and (2.28) as

$$\rho_{a}^{\mathrm{S}} = \frac{\mathcal{M}_{a}(\rho)}{\Pr\left(A_{\mathrm{D}} = a | \rho\right)}, \tag{2.29}$$

$$\Pr\left(A_{\mathrm{D}} = a | \rho\right) = \mathrm{Tr}[\mathcal{M}_{a}(\rho)]. \tag{2.30}$$

Hence, the general quantum measurement is given by the set of the maps $\{\mathcal{M}_a\}_a$, whose elements are given by the equation (2.27) in the indirect measurement model. Note that the corresponding non-selective measurement is given by the map

$$\mathcal{M} := \sum_a \mathcal{M}_a, \tag{2.31}$$

which is a TPCP map satisfying the those properties on the page 6. Because the map (2.31) is given by

$$\mathcal{M}(\rho) = \mathrm{Tr}\big[U(\rho \otimes \sigma_{\mathrm{D}})U^{\dagger}\big], \tag{2.32}$$

it clearly denotes a general quantum dynamics in the section (2.10).

The quantum measurement $\{\mathcal{M}_a\}_a$ is mathematically called a CP instrument. The CP instrument is a set of completely positive (CP) linear maps whose sum is a TPCP map. Similarly to the general quantum dynamics of the section 2.1.2, an arbitrary CP instrument can be represented as an indirect measurement model.

The CP instrument has the Kraus representation similarly to the TPCP map. The Kraus representation of the CP instrument is given as follows: for a CP instrument $\{\mathcal{M}_a\}_a$, the each CP map $\mathcal{M}_a$ can be represented by a set of linear operators $\{M_{a,n}\}_n$ satisfying $\sum_n M_{n,a}^{\dagger} M_{n,a} \le I$ and $\sum_{a,n} M_{a,n}^{\dagger} M_{a,n} = I$, where I is the identity operator, such that

$$\mathcal{M}_a(\rho) = \sum_n M_{a,n} \rho M_{a,n}^{\dagger}. \tag{2.33}$$

We thereby obtain the probability (2.30) in the form

$$\Pr(A_{\mathrm{D}} = a|\rho) = \sum_n \mathrm{Tr}\big[M_{a,n} \rho M_{a,n}^{\dagger}\big]. \tag{2.34}$$

In particular, when the echo CP map $\mathcal{M}_a$ of the CP instrument is represented by only one operator M_a, namely

$$\mathcal{M}_a(\rho) = M_a \rho M_a^{\dagger} \tag{2.35}$$

for all outcome a, we call the operator M_a the measurement operator. When the measurement operator is a projection, the equation (2.35) becomes a projection measurement.

Finally, we show a POVM (positive operator valued measure of probability operator valued measure) measurement, which is a quantum measurement focused on a probability of outcomes, ignoring a post-measurement state.

The POVM measurement of the physical quantity A is given by a set of positive Hermitian operators $\{E_a\}_a$ with the normalization $\sum_a E_a = I$. Then, we define the probability $\Pr(A = a|\rho)$ of an outcome a given a state ρ as

$$\Pr(A = a|\rho) := \mathrm{Tr}[E_a \rho]. \tag{2.36}$$

The POVM measurement is an extension of the Born rule (2.19) and satisfies an affine property:

$$\Pr(A = a|p\rho_1 + (1-p)\rho_2) = p\Pr(A = a|\rho_1) + (1-p)\Pr(A = a|\rho_2) \tag{2.37}$$

for any states ρ_1 and ρ_2 with a real number $p \in [0,1]$. On the other hand, the POVM measurement can be derived from the affine property (2.37) [108].

The POVM measurement can be represented by the indirect measurement model, the CP instrument and the Kraus representation. From the equations (2.25), (2.30) and (2.34), we obtain

$$\begin{aligned} E_a &= \mathrm{Tr}_\mathrm{D}\big[U^\dagger(I_\mathrm{S} \otimes P_a^\mathrm{D})U(I_\mathrm{S} \otimes \sigma_\mathrm{D})\big] && (2.38) \\ &= \mathcal{M}_a^\dagger(I_\mathrm{S}) && (2.39) \\ &= \sum_n M_{a,n}^\dagger M_{a,n}, && (2.40) \end{aligned}$$

where $\mathcal{M}_a^\dagger$ is the adjoint of $\mathcal{M}_a$ as defined in the appendix A.

2.2.3 Continuous measurement

Let us consider measurement of a physical quantity A in a closed quantum system. We keep measuring it continuously between time 0 and τ and obtain a measurement record $[a] := \{\, a(t) \mid t \in (0,\tau) \,\}$, where $a(t)$ is a path of the measurement outcome. We call this procedure the continuous measurement.

We approximate the continuous measurement by a series of instantaneous measurements, which we describe as CP instruments $\{\, \mathcal{M}_{a,t} \,\}_a$ of the physical quantity A for each time t [17, 75]. The time evolution between successive two instrument measurements $\{\, \mathcal{M}_{a,t} \,\}_a$ and $\{\, \mathcal{M}_{a,s} \,\}_a$ $(t \leq s)$ is the unitary evolution map $\mathcal{U}_{s,t}$ given by $\mathcal{U}_{s,t}(\rho) := U(s,t)\rho U^\dagger(s,t)$ for an arbitrary state ρ, where $U(s,t)$ is a unitary operator of evolution between time t to s.

We define the continuous-measurement map $\mathcal{M}_{[a]}$ as the limitation of a series of represented instantaneous measurements in the form

$$\begin{aligned} \mathcal{M}_{[a]} := \lim_{N\to\infty} \mathcal{U}_{t_N,t_{N-1}}\, \mathcal{M}_{a_{N-1},t_{N-1}}\, \mathcal{U}_{t_{N-1},t_{N-2}}\, \mathcal{M}_{a_{N-2},t_{N-2}} \\ \times \cdots \times \mathcal{U}_{t_2,t_1}\, \mathcal{M}_{a_1,t_1}\, \mathcal{U}_{t_1,t_0}, \quad (2.41) \end{aligned}$$

where $t_n := n\tau/N$ and $a_n := a(t_n)$. The set of the continuous-measurement maps $\{\, \mathcal{M}_{[a]} \,\}_{[a]}$ is a CP instrument, because the map $\mathcal{M}_{[a]}$ is a CP map and its path integral over all measurement records $[a]$ is trace preserving:

$$\mathrm{Tr}\bigg[\int \mathcal{D}[a]\, \mathcal{M}_{[a]}(\rho)\bigg] = \mathrm{Tr}[\rho] \quad (2.42)$$

for any density matrix ρ, where $\int\mathcal{D}[a]$ denotes a path integral defined by

$$\int \mathcal{D}[a] := \lim_{N\to\infty} \prod_{n=1}^{N-1} \sum_{a_n} . \quad (2.43)$$

Hence, the probability $P([a]\|\rho)$ of a measurement record $[a]$ given a state ρ is given by

$$P([a]\|\rho) := \mathrm{Tr}\big[\mathcal{M}_{[a]}(\rho)\big] \quad (2.44)$$

with

$$\int \mathcal{D}[a]\, P([a]\|\rho) = 1. \tag{2.45}$$

Chapter 3

Time-dependent Hamiltonian approach on conventional studies

One of the important points of thermodynamics is to distinguish the work and the heat in the energy transferred from a system to another. In macroscopic thermodynamics, the work is the energy transferred by varying external parameters of a thermodynamic system, such as the volume and a magnetic field, whereas the heat is the energy transferred by thermal contact with heat baths [10]. However, quantum mechanics itself does not make the distinction of the work and the heat. To construct quantum thermodynamic, it is critical to know how to define the work and the heat quantum-mechanically.

In this chapter, we review a conventional approach to the definition of the work and the heat in quantum thermodynamics by using a time-dependent Hamiltonian.

3.1 Time-dependent Hamiltonian and first law of thermodynamics

In the conventional studies of quantum thermodynamics, a thermodynamic system operated by an external agent is represented by a time-dependent Hamiltonian. This time dependence is derived from the time variation of external parameters of the system which is caused by the operations of an external agent.

In this section, we define the work and the heat from the time-dependent Hamiltonian and derive the first law of thermodynamics.

3.1.1 Work, heat, and first law of the thermodynamics

Let $H(t)$ and $\rho(t)$ denote the time-dependent Hamiltonian of a driven system and its state at time t, respectively. The change of the internal energy ΔU of the driven system from the time $t = 0$ to τ is given by

$$\Delta U = \mathrm{Tr}[\rho(\tau)H(\tau)] - \mathrm{Tr}[\rho(0)H(0)]. \tag{3.1}$$

Since the work is the energy transferred owing to the change of the external parameters and the heat is the energy transferred without the variation of the Hamiltonian, we define the average work performed by the system and the average heat absorbed by it as

$$\langle W\rangle := -\int_0^\tau dt\,\mathrm{Tr}\big[\rho(t)\dot{H}(t)\big], \tag{3.2}$$

$$\langle Q\rangle := \int_0^\tau dt\,\mathrm{Tr}[\dot{\rho}(t)H(t)], \tag{3.3}$$

respectively [8, 9, 27, 32, 36, 39, 42, 52, 68, 85, 116].

These definitions satisfy the first law of thermodynamic, namely the energy conservation. Indeed, deforming the equation (3.1) using derivation with respect to the time t, we obtain

$$\begin{aligned} \Delta U &= \int_0^\tau dt\,\frac{d}{dt}\mathrm{Tr}[\rho(t)H(t)] && (3.4)\\ &= \int_0^\tau dt\,\big(\mathrm{Tr}[\dot{\rho}(t)H(t)] + \mathrm{Tr}\big[\rho(t)\dot{H}(t)\big]\big). && (3.5) \end{aligned}$$

Combining equations (3.2), (3.3) and (3.5), we obtain the energy conservation law in the form of

$$\Delta U = \langle Q\rangle - \langle W\rangle\,. \tag{3.6}$$

Notice that the equation of the motion with respect to the state $\rho(t)$ is irrelevant in the definitions (3.2) and (3.3). In other wards, we can apply them both to closed and open quantum systems.

For example, consider the adiabatic dynamics of a closed quantum system for the driven system $H(t)$. The evolution of the state $\rho(t)$ depends only on the Hamiltonian $H(t)$, and hence follows the von Neumann equation

$$i\hbar\frac{\partial\rho(t)}{\partial t} = [H(t),\rho(t)]\,. \tag{3.7}$$

Calculating the average heat (3.3) using the von Neumann equation (3.7), we obtain

$$\begin{aligned} \langle Q\rangle &= \frac{i}{\hbar}\int_0^\tau dt\,\mathrm{Tr}[[H(t),\rho(t)]\,H(t)] && (3.8)\\ &= \frac{i}{\hbar}\int_0^\tau dt\,(\mathrm{Tr}[H(t)\rho(t)H(t)] - \mathrm{Tr}[\rho(t)H(t)H(t)]) && (3.9)\\ &= 0. && (3.10) \end{aligned}$$

Therefore, the change of the internal energy is equal to the average work:

$$\Delta U = -\langle W\rangle\,. \tag{3.11}$$

3.1.2 Thermodynamics system with heat baths

In the discussion above, the heat baths are represented by the influence on the driven system except for the external parameters. However, some studies [25, 46, 56, 57, 63, 69, 95, 103, 106] of quantum thermodynamics consider the closed quantum system including the driven system and the heat baths. In this approach, we assume that the Hamiltonians of the heat baths do not change in time, and the work performed by the driven system and the heat absorbed by it are equal to the energy decrements of the composite system and the heat bath, respectively. We can thereby derive the first law of thermodynamics.

For simplicity, we consider the case of one heat bath and that the external operation is performed from time 0 to τ. Let $H_{\mathrm{S}}(t)$, H_{B} and $V(t)$ denote the Hamiltonians of the driven system, the heat bath and the interaction between the two systems, respectively. The Hamiltonian $H_{\mathrm{S}}(t)$ of the driven system has time dependence with respect to the external operation. On the other hand, the Hamiltonian H_{B} of the heat bath does not depend on time. We assume that the interaction Hamiltonian $V(t)$ vanishes except during the external operation; $V(t) = 0$ for $t \notin (0, \tau)$. Hence, the Hamiltonian of the composite system is given by

$$H_{\mathrm{tot}}(t) := H_{\mathrm{S}}(t) + V(t) + H_{\mathrm{B}}. \tag{3.12}$$

Let us first find the heat absorbed by the driven system. Since we assume that the composite system is a closed quantum system, the state $\rho(t)$ of the composite system follows the von Neumann equation with respect to the Hamiltonian (3.12) of the composite system. Hence, the average heat of the composite system is zero (see equation (3.10)), and we obtain

$$\begin{aligned} \langle Q \rangle_{\mathrm{S}} := \int_0^{\tau} dt\, \mathrm{Tr}[\dot{\rho}(t)(H_{\mathrm{S}}(t) + V(t))] &= -\int_0^{\tau} dt\, \mathrm{Tr}[\dot{\rho}(t) H_{\mathrm{B}}] && (3.13) \\ &= \mathrm{Tr}[\rho(0) H_{\mathrm{B}}] - \mathrm{Tr}[\rho(\tau) H_{\mathrm{B}}]. && (3.14) \end{aligned}$$

The left-hand side of the above equality denotes the average heat absorbed by the driven system including the contribution of the interaction, and the right-hand side is the energy decrements of the heat bath. Thus, the energy decrements of the heat bath is equal to the heat absorbed by the driven system.

Next, we find the work performed by the driven system. Since the composite system is a closed system, the energy decrement of the composite system is equal to the average work performed by *the composite system* (see equation (3.11)):

$$\mathrm{Tr}[\rho(0) H_{\mathrm{tot}}(0)] - \mathrm{Tr}[\rho(\tau) H_{\mathrm{tot}}(\tau)] = \int_0^{\tau} dt\, \mathrm{Tr}\big[\rho(t) \dot{H}_{\mathrm{tot}}(t)\big]. \tag{3.15}$$

From $\dot{H}_{\mathrm{tot}}(t) = \dot{H}_{\mathrm{S}}(t) + \dot{V}(t)$, we obtain

$$\mathrm{Tr}[\rho(0) H_{\mathrm{tot}}(0)] - \mathrm{Tr}[\rho(\tau) H_{\mathrm{tot}}(\tau)] = \int_0^{\tau} dt\, \mathrm{Tr}\big[\rho(t)\big(\dot{H}_{\mathrm{S}}(t) + \dot{V}(t)\big)\big] =: \langle W \rangle_{\mathrm{S}}\,. \tag{3.16}$$

The right-hand side of the above equality indicates the average work performed by the driven system including contribution of the interaction. Thus, the energy decrements of the composite system is equal to the work performed by the driven system.

Moreover, we define the change of the driven system including contribution of the interaction as

$$\Delta U_{\mathrm{S}} := \mathrm{Tr}[\rho(\tau)(H_{\mathrm{S}}(\tau) + V(\tau))] - \mathrm{Tr}[\rho(0)(H_{\mathrm{S}}(0) + V(0))]. \tag{3.17}$$

We then arrive at the first law of thermodynamics for the driven system:

$$\Delta U_{\mathrm{S}} = \langle Q \rangle_{\mathrm{S}} - \langle W \rangle_{\mathrm{S}}. \tag{3.18}$$

3.2 Second law of thermodynamics

The second law of thermodynamics represents the irreversibility, which is a characteristic and important phenomenon in thermodynamics. To represent the irreversibility, we define the (thermodynamic) entropy S_{th} from a reversible thermodynamic process and obtain the following statement: the entropy change ΔS_{th} of any thermodynamic process satisfies

$$\Delta S_{\mathrm{th}} \geq \sum_n \frac{Q_n}{T_n}, \tag{3.19}$$

where Q_n is the heat absorbed by the nth heat bath at a temperature T_n. This is well known as the Clausius inequality, which is one of the statement of the second law.

Another representation of the second law of thermodynamics is focused on the extracted work. It is known as the principle of maximum work: the extracted work under any isothermal process is maximal for a reversible isothermal process. To represent the maximum work, we define the Helmholtz free energy as $F^{\mathrm{eq}} := U - TS_{\mathrm{th}}$, where U and T are an internal energy and an temperature, respectively. Then, the maximum work is represented by the difference of the Helmholtz free energies. Hence, the principle of maximum work is given by

$$W \leq -\Delta F^{\mathrm{eq}}, \tag{3.20}$$

where W and ΔF^{eq} are the extracted work under any isothermal process and the difference of the Helmholtz free energies between the initial and the final equilibriums, respectively.

In macroscopic dynamics, the equations of motion have the reversibility. Deriving the irreversibility of thermodynamics from this microreversibility is an important issue of statistical physics, and has been studied by many researches.

In this section, we derive the second law of thermodynamic for quantum systems using the time-dependent Hamiltonian approach.

3.2.1 Clausius inequality and entropy production

In quantum thermodynamic, we define the (nonequilibrium) entropy of the state ρ with the von Neumann entropy

$$S(\rho) := -\mathrm{Tr}\big[\rho \log \rho\big]. \tag{3.21}$$

This definition comes from the analogy of (equilibrium) statistical mechanics, and is equal to the thermodynamic entropy except for the Boltzmann constant when the state is in the equilibrium. Because the von Neumann entropy is unitary invariant, it does not change in the closed quantum system.

The second law of thermodynamics is represented as

$$\Delta S \geq \sum_n \beta_n \langle Q_n \rangle , \tag{3.22}$$

where ΔS is the change of the von Neumann entropy of the driven system and $\langle Q_n \rangle$ is the average heat that the driven system absorbs from the nth heat bath at the inverse temperature β_n. This is a representation of the Clausius inequality in quantum thermodynamics.

In nonequilibrium thermodynamics, the second law is often represented in another form using the entropy production. The entropy production is the entropy produced inside the driven system and is given by

$$\Delta_{\mathrm{i}} S := \Delta S - \sum_n \beta_n \langle Q_n \rangle . \tag{3.23}$$

From the equation (3.22), we have the second law in terms of the non-negativity of the entropy production:

$$\Delta_{\mathrm{i}} S \geq 0. \tag{3.24}$$

The non-negativity of the entropy production has been shown in several situations [9, 56]. In this section, we show it in the case of the section 3.1.2, for the Hamiltonian (3.12). Let $\rho_{\mathrm{S}}(t)$ denote the state of the driven system derived from the trace of $\rho(t)$ over the degrees of the heat bath. We assume that the initial state $\rho(0)$ of the composite system does not have entanglement between the driven system and the heat bath, and the initial state of the heat bath is the canonical distribution at an inverse temperature β:

$$\rho(0) = \rho_{\mathrm{S}}(0) \otimes \rho_{\mathrm{B}}^{\mathrm{eq}}, \quad \rho_{\mathrm{B}}^{\mathrm{eq}} := \frac{e^{-\beta H_{\mathrm{B}}}}{\mathrm{Tr}\big[e^{-\beta H_{\mathrm{B}}}\big]}. \tag{3.25}$$

Since the composite system is closed, its entropy does not change:

$$\begin{aligned} S(\rho(\tau)) = S(\rho(0)) &= -\mathrm{Tr}\big[\rho_{\mathrm{S}}(0) \log \rho_{\mathrm{S}}(0)\big] - \mathrm{Tr}\big[\rho_{\mathrm{B}}^{\mathrm{eq}} \log \rho_{\mathrm{B}}^{\mathrm{eq}}\big] && (3.26) \\ &= S(\rho_{\mathrm{S}}(0)) - \mathrm{Tr}\big[\rho_{\mathrm{B}}^{\mathrm{eq}} \log \rho_{\mathrm{B}}^{\mathrm{eq}}\big], && (3.27) \end{aligned}$$

from which we obtain the change of the entropy of the driven system in the form

$$\begin{aligned} \Delta S &:= S(\rho_{\mathrm{S}}(\tau)) - S(\rho_{\mathrm{S}}(0)) && (3.28) \\ &= S(\rho_{\mathrm{S}}(\tau)) - S(\rho(\tau)) - \mathrm{Tr}\big[\rho_{\mathrm{B}}^{\mathrm{eq}} \log \rho_{\mathrm{B}}^{\mathrm{eq}}\big] && (3.29) \\ &= -\mathrm{Tr}\big[\rho_{\mathrm{S}}(\tau) \log \rho_{\mathrm{S}}(\tau)\big] + \mathrm{Tr}\big[\rho(\tau) \log \rho(\tau)\big] - \mathrm{Tr}\big[\rho_{\mathrm{B}}^{\mathrm{eq}} \log \rho_{\mathrm{B}}^{\mathrm{eq}}\big]. && (3.30) \end{aligned}$$

On the other hand, from the equation (3.14), we obtain the average heat absorbed by the driven system S as

$$\begin{aligned} \beta \langle Q \rangle_{\mathrm{S}} &= \beta\big(\mathrm{Tr}\big[\rho_{\mathrm{B}}^{\mathrm{eq}} H_{\mathrm{B}}\big] - \mathrm{Tr}\big[\rho(\tau) H_{\mathrm{B}}\big]\big) && (3.31) \\ &= \mathrm{Tr}\big[\rho(\tau) \log e^{-\beta H_{\mathrm{B}}}\big] - \mathrm{Tr}\big[\rho_{\mathrm{B}}^{\mathrm{eq}} \log e^{-\beta H_{\mathrm{B}}}\big] && (3.32) \\ &= \mathrm{Tr}\big[\rho(\tau) \log \rho_{\mathrm{B}}^{\mathrm{eq}}\big] - \mathrm{Tr}\big[\rho_{\mathrm{B}}^{\mathrm{eq}} \log \rho_{\mathrm{B}}^{\mathrm{eq}}\big]. && (3.33) \end{aligned}$$

Therefore, the entropy production (3.23) is reduced to

$$\begin{aligned}\Delta_{\mathrm{i}}S &:= \Delta S - \beta\langle Q\rangle_{\mathrm{S}} && (3.34)\\ &= -\mathrm{Tr}\big[\rho(\tau)\log\big(\rho_{\mathrm{S}}(\tau)\otimes\rho_{\mathrm{B}}^{\mathrm{eq}}\big)\big] + \mathrm{Tr}\big[\rho(\tau)\log\rho(\tau)\big] && (3.35)\\ &= D\Big(\rho(\tau)\Big\|\rho_{\mathrm{S}}(\tau)\otimes\rho_{\mathrm{B}}^{\mathrm{eq}}\Big), && (3.36)\end{aligned}$$

where $D(\rho\|\sigma) := \mathrm{Tr}\big[\rho\log\rho\big] - \mathrm{Tr}\big[\rho\log\sigma\big]$ is the quantum relative entropy. Because the quantum relative entropy is non-negative [24], we obtain the second law of thermodynamics, the equation (3.24).

3.2.2 Principle of maximum work and free energy

In the previous section, we define the entropy production $\Delta_{\mathrm{i}}S$ as the difference of the absorbed heat from the entropy change. Using the energy conservation law, we can describe the entropy production in terms of the extracted work and derive the principle of maximum work under quantum thermodynamics.

We now assume the case of one heat bath. Then, the energy conservation (3.6) and the entropy production (3.23) reduce to

$$\begin{aligned}\Delta U &= \langle Q\rangle - \langle W\rangle, && (3.37)\\ \Delta_{\mathrm{i}}S &= \Delta S - \beta\langle Q\rangle, && (3.38)\end{aligned}$$

respectively, which are followed by

$$\Delta_{\mathrm{i}}S = \Delta S - \beta\Delta U - \beta\langle W\rangle. \qquad (3.39)$$

In the analogy of the Helmholtz free energy of thermodynamics, let us define the nonequilibrium free energy [57, 63, 69, 76, 111] as

$$F(\rho;H) := \mathrm{Tr}[\rho H] - \beta^{-1}S(\rho). \qquad (3.40)$$

We therefore have

$$\begin{aligned}\Delta F &:= F(\rho(\tau);H(\tau)) - F(\rho(0);H(0)) && (3.41)\\ &= \Delta U - \beta^{-1}\Delta S, && (3.42)\end{aligned}$$

where we used the equation (3.1). We thus obtain the entropy production in terms of the work in the form

$$\Delta_{\mathrm{i}}S = -\beta(\Delta F + \langle W\rangle). \qquad (3.43)$$

The nonequilibrium free energy (3.40) can be characterized by the reversible isothermal process as well as the Helmholtz free energy in thermodynamics. Its difference represents the maximum work between two general state. Indeed, the non-negativity of the entropy production (3.24) and the equation (3.43) give

$$\langle W\rangle \leq -\Delta F. \qquad (3.44)$$

This is the principle of maximum work under quantum thermodynamics.

Finally, we show the relation between the nonequilibrium and Helmholtz free energies. Transforming the definition (3.40) using the canonical distribution at the inverse temperature β,

$$\rho^{\mathrm{eq}}(\beta; H) := \frac{e^{-\beta H}}{Z(\beta; H)} \tag{3.45}$$

with $Z(\beta; H) := \mathrm{Tr}\big[e^{-\beta H}\big]$, we obtain

$$\begin{aligned} F(\rho; H) &= -\beta^{-1}\big(\mathrm{Tr}\big[\rho \log \rho^{\mathrm{eq}}(\beta; H)\big] + \log Z(\beta; H)\big) - \beta^{-1}\mathrm{Tr}\big[\rho \log \rho\big] && (3.46)\\ &= -\beta^{-1} \log Z(\beta; H) + \beta^{-1} D(\rho \| \rho^{\mathrm{eq}}(\beta; H)), && (3.47) \end{aligned}$$

where $D(\rho\|\sigma) := \mathrm{Tr}\big[\rho \log \rho\big] - \mathrm{Tr}\big[\rho \log \sigma\big]$ is the quantum relative entropy. The first term is the Helmholtz free energy $F^{\mathrm{eq}}(\beta; H) := -\beta^{-1} \log Z(\beta; H)$. The non-negativity of the quantum relative entropy in the second term therefore gives

$$F(\rho; H) - F^{\mathrm{eq}}(\beta; H) = \beta^{-1} D(\rho \| \rho^{\mathrm{eq}}(\beta; H)) \geq 0. \tag{3.48}$$

Thus, the nonequilibrium free energy is always greater than the Helmholtz at the same temperature, and is equal to it when the state is at equilibrium.

In particular, if the initial state is the canonical distribution $\rho^{\mathrm{eq}}(\beta; H(0))$, the nonequilibrium free energy is equal to the Helmholtz one: $F(\rho^{\mathrm{eq}}(\beta; H(0)); H(0)) = F^{\mathrm{eq}}(\beta; H(0))$. Using the equations (3.44) and (3.48), we can obtain a quantum counterpart of the equation (3.20):

$$\begin{aligned} \langle W \rangle &\leq F(\rho^{\mathrm{eq}}(\beta; H(0)); H(0)) - F(\rho(\tau); H(\tau)) && (3.49)\\ &= F^{\mathrm{eq}}(\beta; H(0)) - F^{\mathrm{eq}}(\beta; H(\tau)) =: -\Delta F^{\mathrm{eq}}. && (3.50) \end{aligned}$$

3.2.3 Second law of thermodynamics with information

Macroscopic thermodynamics focuses on macroscopic systems and gives universal laws without depending on microscopic details of thermodynamic systems. In order to derive this property from microscopic mechanics, we calculate statistical properties of the collection of many particles in the thermodynamic system, not the motion of each particle. If we can know the motion of each particle, can we obtain the thermodynamic laws?

To this question, Maxwell, in 1871, considered a thought experiment in which an agent performs measurements on each particle and make operations on the thermodynamic system depending on the measurement results. He thus showed that the second law of thermodynamics is a stochastic law derived from statistical properties [2]. He demonstrated that this agent can separate gas at a certain temperature into two boxes of gas at different temperatures without affecting the gas, and claimed that the second law of thermodynamics was therefore broken. At the present time, this agent is called *Maxwell's demon* and the breaking of the second law of thermodynamics is called *the paradox of Maxwell's demon*. It is one of the most important topics in thermodynamics [29, 53].

Many researchers have studied to understand and solve this paradox. Particularly, Landauer's principle [5] is the most famous. Landauer's principle claims that any logical irreversibility, such as the erasure process of information, corresponds to the thermodynamic irreversibility and increases the corresponding entropy. Bennett, in 1982, applied this principle to the paradox of Maxwell's demon, and solved the paradox [11]. Because a physically possible demon cannot store information limitlessly, it can increase the entropy. Thus, the composite system of a thermodynamic system and the demon obeys the second law of thermodynamics.

After the solution of the paradox using Landauer's principle, researchers have studied Maxwell's demon in more detail; this research field is called *information thermodynamics*. Today, we know an extended second law, called the second law of information thermodynamics, in the following form [46, 50, 80–82]: When the initial state of a thermodynamic system is the canonical distribution at an inverse temperature β, the average work $\langle W\rangle$ performed by the thermodynamic system satisfies

$$\langle W\rangle \leq -\langle \Delta F^{\mathrm{eq}}\rangle + \beta^{-1} I, \tag{3.51}$$

where $\langle \Delta F^{\mathrm{eq}}\rangle$ is the average change of the Helmholtz free energy and I is the amount of information obtained by the demon from the thermodynamic system. When the thermodynamic system is a classical system, the amount of information I is the mutual information between the system and the demon, while for a quantum system, the amount I is the information gain by the quantum measurement, which is defined by Groenewold [6] and Ozawa [12] and is called QC-mutual information by Sagawa and Ueda [46].

As we can see in the equation (3.51), the upper limit of the extracted work exceeds the one in the second law of thermodynamics by the amount of information I. Indeed, for the (classical) Szilard engine [3], which is a famous model of Maxwell's demon, we have $\langle W\rangle = \beta^{-1}\log 2$, $\Delta F^{\mathrm{eq}} = 0$, and $I = \log 2$. Hence, the work of the Szilard engine breaks the conventional second law and achieves the equality of (3.51). The quantum version of the Szilard engine functions in the same way [70].

Let us now regard Maxwell's demon as a thermodynamic system and find inequalities regarding the quantities of the demon. Let $\langle W\rangle_{\mathrm{meas}}$ and $\langle W\rangle_{\mathrm{eras}}$ denote the average work required by the measurement and the information erasure of the demon, respectively, We find the second laws of information thermodynamics with respect to the demon in the following form [54]:

$$\langle W\rangle_{\mathrm{meas}} \geq \left\langle \Delta F^{\mathrm{eq}}_{\mathrm{demon}}\right\rangle - \beta^{-1}(H - I), \tag{3.52}$$

$$\langle W\rangle_{\mathrm{eras}} \geq -\left\langle \Delta F^{\mathrm{eq}}_{\mathrm{demon}}\right\rangle + \beta^{-1} H, \tag{3.53}$$

where $\left\langle \Delta F^{\mathrm{eq}}_{\mathrm{demon}}\right\rangle$ is the average change of the Helmholtz free energy of the demon and H is the Shannon entropy regarding the measurement outcome.

Combining the above three equations (3.51), (3.52) and (3.53), we obtain

$$\langle W\rangle - \langle W\rangle_{\mathrm{meas}} - \langle W\rangle_{\mathrm{eras}} \leq -\langle \Delta F^{\mathrm{eq}}\rangle . \tag{3.54}$$

Hence, we thus recover the second law of thermodynamics for the combined system of the thermodynamic system and the demon.

In this way, we obtain a relation between the thermodynamics and the information from the feedback operation, an operation that depends on the measurement outcome of the thermodynamic system, which is nothing but what Maxwell's demon. The amount of information in the equations (3.51), (3.52) and (3.53) is large when the probability of the measurement outcome has wide tails. Because a microscopic system fluctuates larger than a macroscopic one, the second law of information thermodynamics is important in the microscopic system.

In quantum systems, we can derive the three versions of the second law, (3.51), (3.52) and (3.53) using the entanglement [93–95, 103]. To understand quantum thermodynamics, it is not important only the relation of the information but also the entanglement.

3.3 Fluctuation theorems

From statistical mechanics, we know that the state of a system fluctuates. This fluctuation is small when the system size is large enough. Thus, we have no problem in deriving macroscopic thermodynamics. When we consider thermodynamics in microscopic systems, on the other hand, we cannot ignore the fluctuation. Are there rules that govern the fluctuation? The fluctuation theorem indeed is a statement for physical quantities in nonequilibrium processes, such as the work, the heat and the entropy production.

A typical form of the fluctuation theorem is given by the following equation on the probability $p_{\mathrm{F}}(\Omega)$ of a thermodynamic quantity Ω in a nonequilibrium process [66, 83]:

$$p_{\mathrm{F}}(\Omega) = e^{a(\Omega-b)} p_{\mathrm{B}}(-\Omega), \tag{3.55}$$

where a and b are appropriate constants and $p_{\mathrm{B}}(\Omega)$ is the probability for the backward process. For example, the work performed by a thermodynamics system satisfies the work fluctuation relation

$$p_{\mathrm{F}}(W) = e^{-\beta(W+\Delta F^{\mathrm{eq}})} p_{\mathrm{B}}(-W), \tag{3.56}$$

where β is the inverse temperature and ΔF^{eq} is the change of the Helmholtz free energy of the thermodynamic system. This work fluctuation relation is called Crooks' fluctuation theorem [18].

The fluctuation theorem stochastically permits the quantities to violate the second law of thermodynamics. In the case of Crooks' fluctuation theorem [18], the work beyond the principle of maximum work $W \leq -\Delta F^{\mathrm{eq}}$ occurs with a non-zero probability.

The expectation with respect to the probability $p_{\mathrm{F}}(\Omega)$ of the fluctuation theorems (3.55) gives

$$\left\langle e^{-a(\Omega-b)} \right\rangle := \int d\Omega\, p_{\mathrm{F}}(\Omega) e^{-a(\Omega-b)} = 1. \tag{3.57}$$

The above equation is also a kind of the fluctuation theorem, and is called the integral fluctuation theorem [83]. Particularly when the quantity Ω is the work W, we obtain

$$\left\langle e^{\beta W} \right\rangle = e^{-\beta \Delta F^{\mathrm{eq}}}, \tag{3.58}$$

which is called the Jarzynski equality [14]. Applying the Jensen inequality $\langle e^f \rangle \geq e^{\langle f \rangle}$ to the Jarzynski equality, we obtain

$$\langle W \rangle \leq -\Delta F^{\mathrm{eq}}. \tag{3.59}$$

In other words, the second law holds for the expectation value.

The fluctuation theorem has been theoretically derived in various situations [14–16, 18–20, 22, 23, 25, 27, 28, 30, 31, 34, 35, 37, 38, 40–42, 44, 45, 47–49, 55, 58, 60, 61, 64, 66, 67, 71, 77, 78, 83, 84, 86–88, 91, 92, 99–101, 104, 106, 107, 109, 112, 113, 118] and have been experimented in various microscopic systems [33, 59, 65, 72, 90, 97, 98]. In the following, we show a quantum version of the fluctuation theorem, particularly the work fluctuation relations [23, 25, 30, 40, 48].

3.3.1 Work fluctuation relations

We show a quantum version of the fluctuation theorem with respect to the work.

To consider the work fluctuation, we define the work extracted by a single operation, not the average work. Kurchan [23] and Tasaki [25] defined the work in a single operation as the difference of the outcomes of two energy measurements.

We now consider a closed quantum system with the time-dependent Hamiltonian $H(t)$. The instantaneous spectral decomposition of $H(t)$ is given by

$$H(t) = \sum_n E_n(t) P_n(t), \tag{3.60}$$

where $E_n(t)$ is the energy eigenvalue at each time and $P_n(t)$ is the corresponding eigenprojection.

We assume the work extraction preformed from time 0 to τ. Then we consider the following process:

1. The initial state is the equilibrium state at the inverse temperature β, namely, is given by
$$\rho_0^{\mathrm{can}} := \frac{e^{-\beta H(0)}}{Z_0} \tag{3.61}$$
with $Z_0 := \mathrm{Tr}\left[e^{-\beta H(0)}\right]$.

2. We measure the energy of the driven system using the energy projection $P_n(0)$. We assume that the energy outcome is $E_n(0)$.

3. After the energy measurement, we let the driven system evolve from time 0 to τ. This time evolution is given by the unitary operator
$$U := \mathbb{T} \exp\left(-\frac{i}{\hbar} \int_0^\tau dt\, H(t)\right), \tag{3.62}$$
where $\mathbb{T}$ is time ordering.

4. Finally, we measure the energy of the driven system using the energy projection $P_m(\tau)$ and assume that the energy outcome is $E_m(\tau)$.

For the above process, we obtain the joint probability of the two specific energy outcomes $E_n(0)$ and $E_m(\tau)$ in the form

$$p_{n,m} := \frac{e^{-\beta E_n(0)}}{Z_0} \mathrm{Tr}\big[P_m(\tau) U P_n(0) U^\dagger\big]. \tag{3.63}$$

Accordingly to the energy conservation law, we assume that the extracted work is equal to the energy loss of the driven system. Then, the probability distribution of the extracted work W in this process is given by

$$\begin{aligned} p_{\mathrm{F}}(W) &:= \sum_{n,m} \delta(W - E_n(0) + E_m(\tau)) p_{n,m} && (3.64)\\ &= \sum_{n,m} \delta(W - E_n(0) + E_m(\tau)) \frac{e^{-\beta E_n(0)}}{Z_0} \mathrm{Tr}\big[P_m(\tau) U P_n(0) U^\dagger\big], && (3.65)\end{aligned}$$

where $\delta(x)$ is the delta function. Using the property of the delta function $\delta(x - x_0) f(x) = \delta(x - x_0) f(x_0)$ and the cyclic property of the trace, we obtain

$$p_{\mathrm{F}}(W) = \frac{Z_\tau}{Z_0} e^{-\beta W} \sum_{n,m} \delta(W - E_n(0) + E_m(\tau)) \frac{e^{-\beta E_m(\tau)}}{Z_\tau} \mathrm{Tr}\big[P_n(0) U^\dagger P_m(\tau) U\big], \tag{3.66}$$

where $Z_\tau := \mathrm{Tr}\big[e^{-\beta H(\tau)}\big]$.

The summand in the equation (3.66) is the probability distribution of the work when the initial state is the canonical distribution of the final Hamiltonian $H(\tau)$ and the time evolution is the unitary operator $U^\dagger$, which is a backward time evolution. Let us define the backward probability distribution of the work as

$$p_{\mathrm{B}}(W) := \sum_{n,m} \delta(W - E_m(\tau) + E_n(0)) \frac{e^{-\beta E_m(\tau)}}{Z_\tau} \mathrm{Tr}\big[P_n(0) U^\dagger P_m(\tau) U\big]. \tag{3.67}$$

We thereby obtain

$$p_{\mathrm{F}}(W) = e^{-\beta(W + \Delta F^{\mathrm{eq}})} p_{\mathrm{B}}(-W), \tag{3.68}$$

where ΔF^{eq} is the difference of the Helmholtz free energy in the form

$$\Delta F^{\mathrm{eq}} := F^{\mathrm{eq}}_\tau - F^{\mathrm{eq}}_0 = -\beta^{-1} \log \frac{Z_\tau}{Z_0} \tag{3.69}$$

with $F^{\mathrm{eq}}_\tau := -\beta^{-1} \log Z_\tau$. This is a quantum version of the fluctuation theorem [23, 26, 48].

Calculating the expectation of $e^{\beta W}$, we obtain a quantum version of the Jarzynski equation in the form

$$\langle e^{\beta W} \rangle := \int dW\, p_{\mathrm{F}}(W) e^{\beta W} = e^{-\beta \Delta F^{\mathrm{eq}}}. \tag{3.70}$$

3.3.2 Work fluctuation relation under feedback

Similarly to the argument of Maxwell's demon in the section 3.2.3, we can consider the fluctuation theorems under feedback processes. For simplicity, we show a quantum fluctuation theorem under the feedback process with a classical error. The classical error means that the measurement outcome changes according to a conditional probability.

We consider the following process for a closed quantum system:

1. Let $H(0)$, $E_n(0)$ and $P_n(0)$ denote the initial Hamiltonian, its eigenvalues and the corresponding eigenprojections, respectively. The initial state of the system is the canonical distribution at an inverse temperature β:

$$\rho_0^{\mathrm{eq}} := \frac{e^{-\beta H(0)}}{Z_0} = \sum_n \frac{e^{-\beta E_n(0)}}{Z_0} P_n(0) \tag{3.71}$$

   with $Z_0 := \mathrm{Tr}\left[e^{-\beta H(0)}\right]$. The corresponding Helmholtz free energy is given by $F_0^{\mathrm{eq}} := -\beta^{-1}\log Z_0$.

2. We measure the energy of the system using the projection $P_n(0)$. We assume that the energy outcome is $E_n(0)$.

3. After the energy measurement, we let the system evolve from time 0 to τ_{meas} following the time-dependent Hamiltonian $H(t)$. The time evolution is given by the unitary operator

$$U := \mathbb{T}\exp\left(-\frac{i}{\hbar}\int_0^{\tau_{\mathrm{meas}}} dt\, H(t)\right), \tag{3.72}$$

   where $\mathbb{T}$ is time ordering.

4. At the time τ_{meas}, we perform an intermediate measurement using the projection Π_x and obtain the outcome x.

5. The intermediate measurement outcome x is changed to the outcome y following the conditional probability $p(y|x)$ because of the classical error.

6. After the intermediate measurement, we perform the feedback operation depending on the outcome y. We let the system evolve from time τ_{meas} to τ following the time-dependent Hamiltonian $H_y(t)$ which depends on y; we here implement the feedback operation by means of the y-dependence. Then, the time evolution is given by the unitary operator

$$U_y := \mathbb{T}\exp\left(-\frac{i}{\hbar}\int_{\tau_{\mathrm{meas}}}^{\tau} dt\, H_y(t)\right). \tag{3.73}$$

   The corresponding Helmholtz free energy is given by $F_{t,y}^{\mathrm{eq}} := -\beta^{-1}\log Z_t^{(y)}$ with $Z_t^{(y)} := \mathrm{Tr}\left[e^{-\beta H_y(t)}\right]$.

7. We perform the energy measurement using the eigenprojection $P_m^{(y)}(\tau)$ of the final Hamiltonian $H_y(\tau)$. Assume that we obtain the eigenvalue $E_m^{(y)}(\tau)$ as the energy outcome.

We obtain the probability of the specific outcomes $E_n(0)$, x, y and $E_m^{(y)}(\tau)$ in the form

$$p_{n,x,y,m} := \frac{e^{-\beta E_n(0)}}{Z_0}\mathrm{Tr}\Big[P_m^{(y)}(\tau)U_y\Pi_x U P_n(0)U^\dagger\Pi_x U_y^\dagger\Big]p(y|x). \tag{3.74}$$

Similarly to the section 3.3.1, we define the extracted work as the energy loss of the system:

$$W_{n,y,m} := E_n(0) - E_m^{(y)}(\tau). \tag{3.75}$$

We also define the difference of the Helmholtz free energy and the (non-average) mutual information as

$$\Delta F_y^{\mathrm{eq}} := F_{\tau,y}^{\mathrm{eq}} - F_0^{\mathrm{eq}}, \tag{3.76}$$

$$I_{x,y} := \log p(y|x) - \log p_y \tag{3.77}$$

with $p_y := \sum_{n,x,m} p_{n,x,y,m}$, respectively. Calculating the expectation of $e^{\beta(W_{n,y,m}+\Delta F_y^{\mathrm{eq}})-I_{x,y}}$ with respect to the probability (3.74), we obtain the quantum Jarzynski equality with the (classical) information in the form

$$\Big\langle e^{\beta(W+\Delta F^{\mathrm{eq}})-I}\Big\rangle := \sum_{n,x,y,m} p_{n,x,y,m} e^{\beta(W_{n,y,m}+\Delta F_y^{\mathrm{eq}})-I_{x,y}} \tag{3.78}$$

$$= \sum_{n,x,y,m} \frac{e^{-\beta E_m^{(y)}(\tau)}}{Z_\tau^{(y)}}\mathrm{Tr}\Big[P_m^{(y)}(\tau)U_y\Pi_x U P_n(0)U^\dagger\Pi_x U_y^\dagger\Big]p_y \tag{3.79}$$

$$= \sum_y \mathrm{Tr}\big[\rho_{\tau,y}^{\mathrm{eq}}\big]p_y = 1, \tag{3.80}$$

where $\rho_{\tau,y}^{\mathrm{eq}} := e^{-\beta H_y(\tau)}/Z_\tau^{(y)}$ is the canonical distribution of the final Hamiltonian for the outcome y.

Because we here suppose that the intermediate measurement is the projection with the classical error, the equation (3.80) includes the classical mutual information. In the case of more general quantum measurements [88], the classical mutual information in the equation (3.80) is replaced by an information gain whose expectation is the QC-mutual information in the equation (3.51). Thus, applying the Jensen inequality $\langle e^f\rangle \geq e^{\langle f\rangle}$ to the equation (3.80), we can obtain the second law of information thermodynamics of the equation (3.51).

Moreover, calculating the expectation of $e^{\beta(W_{n,y,m}+\Delta F_y^{\mathrm{eq}})}$, we obtain another type of the quantum Jarzynski equality under the feedback operation in the form

$$\left\langle e^{\beta(W+\Delta F^{\mathrm{eq}})}\right\rangle := \sum_{n,x,y,m} p_{n,x,y,m} e^{\beta\left(W_{n,y,m}+\Delta F_y^{\mathrm{eq}}\right)} \tag{3.81}$$

$$= \sum_{n,x,y,m} \frac{e^{-\beta E_m^{(y)}(\tau)}}{Z_\tau^{(y)}} \mathrm{Tr}\left[P_m^{(y)}(\tau) U_y \Pi_x U P_n(0) U^\dagger \Pi_x U_y^\dagger\right] p(y|x) \tag{3.82}$$

$$= \sum_{x,y} \mathrm{Tr}\left[\Pi_x U_y^\dagger \rho_{\tau,y}^{\mathrm{eq}} U_y \Pi_x\right] p(y|x) =: \gamma. \tag{3.83}$$

Using the Jensen inequality $\left\langle e^f \right\rangle \geq e^{\langle f \rangle}$, we obtain another type of the second law of information thermodynamics in the form

$$\langle W \rangle \leq -\langle \Delta F \rangle + \beta^{-1} \log \gamma. \tag{3.84}$$

The quantity γ characterizes the efficiency of the feedback operation [62] because the extracted work is bounded by it. It has been measured by an experiment in a classical system [65].

Chapter 4

Work extraction as measurement process

In this chapter, we review a new approach of work extraction in quantum thermodynamics instead of the conventional approach using time-dependent Hamiltonian. Our new formulation is based on a quantum measurement process.

4.1 Problems of time-dependent Hamiltonian approach

In the previous chapter, we analyzed quantum thermodynamics using a time-dependent Hamiltonian of a driven system. To define the extracted work, this approach made the following assumptions:

- The time evolution of the thermodynamic system, which is the driven system with heat baths, is described by the unitary operator generated from the time-dependent Hamiltonian of the thermodynamics system.
- The work performed on the external agent is equal to the energy loss of the thermodynamic system.

These assumptions have the following problems. First, the actual dynamics of quantum system is not generally described by a unitary operator. Because the external agent is also a physical system that interacts with the thermodynamic system, the thermodynamic system is an open quantum system. Hence, the dynamics of the thermodynamic system is not generally the unitary evolution. Next, the statistical property of the work given by the external agent is not corresponding to one of the energy loss of the thermodynamic system.

Several studies [93, 114, 117, 119, 122] of these problems, indeed showed that the two assumptions are not compatible with each other. In other words, when the dynamics of the thermodynamic system is described by the unitary evolution, we cannot truly describe the statistical property of the extracted work as the energy loss of the thermodynamic system; see an example of a two-level system in the section 5.1. For that reason, we necessarily describe the work extraction different form the time-dependent Hamiltonian approach.

In order to resolve this problem, we can consider two approaches of the work extraction. One is to introduce an external agent which obtains the work from the thermodynamic system and the other is to consider the work extraction in the framework of quantum measurement theory. In several studies [102, 105] of the first approach, they introduced

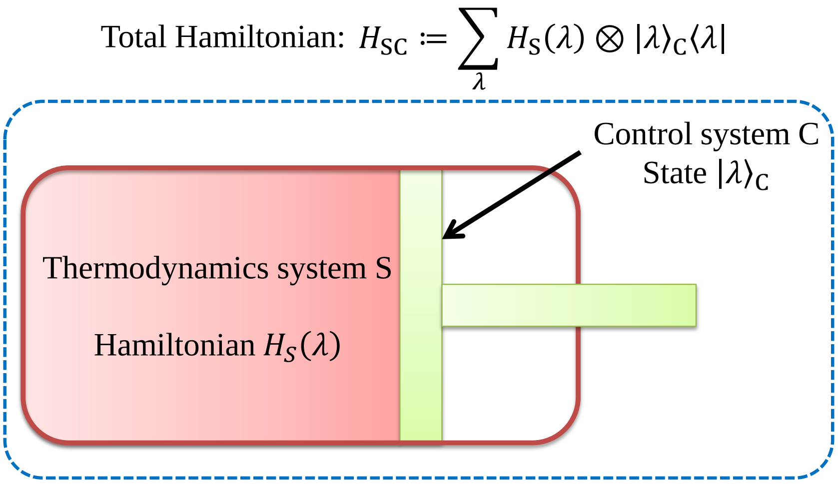

Figure 4.1: Illustration of the thermodynamic system S, such as a gas, controlled by the control system C, such as a piston. The Hamiltonian of the total system is given by the time-independent Hamiltonian H_{SC} defined by the equation (4.1). Whereas the Hamiltonian of the total system does not change in time, one of the thermodynamic system S changes according to the state of the control system C.

a work-storage device, such as a battery, as an external agent that obtains the energy from the thermodynamic system and derived the second law of quantum thermodynamics. On the other hand, in several studies [93, 117] of the other approach, they considered an analogy between the work extraction and a quantum measurement process and introduce a new formulation of the work extraction, which is called the measurement-based work extraction. Note that the two approaches of the work extraction may have a similar relation between an indirect measurement model and a map representation of quantum measurement, because the approach using the work-storage device may reduce to the measurement-based work extraction when the work-storage device is traced out. We adopt the latter in the present thesis and describe it in the present chapter.

4.2 Control system

Instead of the previous approach using the time-dependent Hamiltonian, we use a time-independent Hamiltonian in order to consider the work extraction of quantum thermodynamics. For the actual thermodynamic system, the Hamiltonian clearly seems to change along time. We solve this gap by introducing a control system [89, 93, 105, 110, 117].

Let us assume that the Hamiltonian of the thermodynamic system S depends on a parameter λ as in $H_{\mathrm{S}}(\lambda)$. We define the control system as a quantum system having an orthonormal basis $\{\, |\lambda\rangle_{\mathrm{C}} \,\}_{\lambda}$ corresponding to the value of the parameter λ. The Hamiltonian of the system composed by the thermodynamic system S and the control system C is given by

$$H_{\mathrm{SC}} := \sum_{\lambda} H_{\mathrm{S}}(\lambda) \otimes |\lambda\rangle_{\mathrm{C}}\langle\lambda|. \tag{4.1}$$

Using a cylinder as an example, the thermodynamic system S and the control system C are a gas in the cylinder and its piston, respectively (see the figure 4.1). The Hamiltonian of the thermodynamic system S changes according to the state of the control system C. For example, if the state of the composite system is the direct product of the state ρ_{S} of the thermodynamic system S and the state $|\lambda_0\rangle$ of the control system C, the average energy of the composite system is equal to the average energy of the thermodynamic system $\lambda = \lambda_0$:

$$\mathrm{Tr}\Big[H_{\mathrm{SC}}\big(\rho_{\mathrm{S}} \otimes |\lambda_0\rangle_{\mathrm{C}}\langle\lambda_0|\big)\Big] = \mathrm{Tr}[H_{\mathrm{S}}(\lambda_0)\rho_{\mathrm{S}}]. \tag{4.2}$$

We can thus analyze quantum thermodynamic using the time-independent Hamiltonian of the composite system of the thermodynamic system and the control system.

4.3 Measurement-based work extraction

As an alternative to the approach of time-dependent Hamiltonian, it has been proposed to regard the work extraction as a quantum measurement process [93, 117, 120].

The work extraction in thermodynamics is a process in which an external agent operates a system and obtain quantities of the work, and consequently the state of the system changes. On the other hand, the measurement in quantum mechanics is a process in which an external agent observes a system and obtain physical quantities, and consequently the state of the system changes. Therefore, we can regard the work extraction in quantum thermodynamics as a measurement process obtaining the quantities of the work.

Based on this analogy, we define the work extraction process as a CP instrument $\left\{ \mathcal{K}_j \right\}_j$ corresponding to a set of outcomes of the work $\left\{ w_j \right\}_j$. Hence, the work extraction is represented by the set of the measurement processes and the outcomes $\left\{ \mathcal{K}_j, w_j \right\}_j$. According to the theory of quantum measurement in the section 2.2.2, the probability P_j of the extracted work w_j is given by

$$P_j := \mathrm{Tr}\big[\mathcal{K}_j(\rho)\big], \tag{4.3}$$

where ρ is the state of the thermodynamic system. The average of the extracted work is given by

$$\langle W\rangle := \sum_j w_j P_j = \sum_j w_j \mathrm{Tr}\big[\mathcal{K}_j(\rho)\big]. \tag{4.4}$$

We expect the work extraction to satisfy the first law of thermodynamics, namely, the energy conservation law. We add the energy conservation law to the work extraction $\left\{ \mathcal{K}_j, w_j \right\}_j$ as follows. Suppose that the thermodynamic system is a closed quantum system with a time-independent Hamiltonian H. The energy conservation for the expectation is given by

$$\langle W\rangle = \mathrm{Tr}[\rho H] - \sum_j \mathrm{Tr}\Big[\mathcal{K}_j(\rho)H\Big] \tag{4.5}$$

for all state ρ of the thermodynamic system. Note that it is sufficient for this energy conservation to be satisfied for the expectation; the work extracted by a single operation is not necessarily equal to the energy loss of the thermodynamic system. In other words, the equation (4.5) is a weak condition of the energy conservation for the work extraction $\left\{\mathcal{K}_j, w_j\right\}_j$.

On the other hand, we can consider a strong condition of the energy conservation of the work extraction $\left\{\mathcal{K}_j, w_j\right\}_j$. Let E_n and $|n\rangle$ denote the eigenvalue of the Hamiltonian H and the corresponding eigenstate, respectively. The strong condition of the energy conservation is given by [117]

$$\mathcal{K}_j\big(|n\rangle\langle n|\big) = P_{E_n-w_j}\mathcal{K}_j\big(|n\rangle\langle n|\big)P_{E_n-w_j} \tag{4.6}$$

for all n and j, where $P_E := \sum_{m;E_m=E}|m\rangle\langle m|$. This energy conservation dictates that the transition occurs between the energy eigenstates with the energy loss always equal to the extracted work w_j. Of course, the condition (4.6) satisfies the condition (4.5).

Beside the above conditions, Hayashi and Tajima proposed two other conditions of the energy conservation [117]. The difference in these energy conservation conditions originated in the difference in the state of the external agent and the interaction between two systems.

4.4 Fully quantum model of work extraction

Similar to the setup in the indirect measurement model for the quantum measurement (see the section 2.2.2), we can consider the external agent obtaining the work from a thermodynamic system as a quantum system [93, 117].

We consider the thermodynamic system S and the external agent E with the Hamiltonians H_S and H_E, respectively. Let the spectral decomposition of H_E given by

$$H_\mathrm{E} = \sum_j \varepsilon_j P_j^\mathrm{E}. \tag{4.7}$$

We suppose that the composition of the two systems are a closed quantum systems and its time evolution is given by a unitary operator U.

Let σ_E denotes the initial state of the external agent. The work extraction $\left\{\mathcal{K}_j, w_j\right\}_j$ is given by [117]

$$\mathcal{K}_j(\rho) := \mathrm{Tr}_\mathrm{E}\Big[\big(I_\mathrm{S}\otimes P_j^\mathrm{E}\big)U(\rho\otimes\sigma_\mathrm{E})U^\dagger\Big], \tag{4.8a}$$

$$w_j := \varepsilon_j - \mathrm{Tr}[\sigma_\mathrm{E}H_\mathrm{E}], \tag{4.8b}$$

where ρ and I_S are the initial state and the identity operator of the thermodynamic system S, respectively, and Tr_E denotes the partial trace over the external agent E.

This work extraction (4.8) does not generally satisfy the energy conservation. Thus, we additionally require the energy conservation of the unitary operator U of the work extraction (4.8):

$$[H_{\mathrm{S}} + H_{\mathrm{E}}, U] = 0. \tag{4.9}$$

The work extraction (4.8) thereby satisfies the weak energy conservation (4.5) for an arbitrary initial state σ_{E} of the external agent E. In particular, when the initial state σ_{E} of the external agent E resides in a specific energy eigenspace, the work extraction (4.8) satisfies the strong energy conservation (4.6). Note that the equation (4.9) is a sufficient condition but not a necessary condition of the energy conservations (4.5) or (4.6).

Chapter 5

Quantum Jarzynski equality of measurement-based work extraction

In the previous chapter, we described the problems of the conventional approach of quantum thermodynamics and reviewed the new formulation of work extraction, which is based on a quantum measurement process. What is the difference in applying the new formulation of work extraction from the conventional approach?

In order to show the difference, we derive a quantum version of the Jarzynski equality using the new formulation of work extraction introduced in the chapter 4 instead of using the conventional approach reviewed in the section 3.3.1.

We first demonstrate the problem of the conventional approach using a two-level system. Next, we derive the quantum Jarzynski equality using the new formulation. To derive this, we first consider the case of a cyclic process, and then the case of a non-cyclic process by extending the case of the cyclic process using a control system given in the section 4.2. Finally, we calculate a quantity appearing in the new derivation using a simple system and show its behavior.

The study in this chapter is based on the reference [119] under the present author's collaboration with Dr. H. Tajima and Prof. N. Hatano.

5.1 Example of problem of time-dependent Hamiltonian approach

In this section, we exemplify the problem of time-dependent Hamiltonian approach using a toy model. We show that energy loss of a thermodynamic system and energy obtained by an external agent have difference behaviors of statistical when we approximate the time evolution of the thermodynamic system to a unitary one. Specifically, we compare variances of both energy changes.

We consider that a thermodynamic system S is a two-level system in which a cyclic process is performed by an external agent E. The cyclic process means that the final Hamiltonian of the thermodynamic system S is equal to the initial one. Let H_{S} and H_{E} denote the (initial) Hamiltonians of the thermodynamic system S and the external agent E, respec-

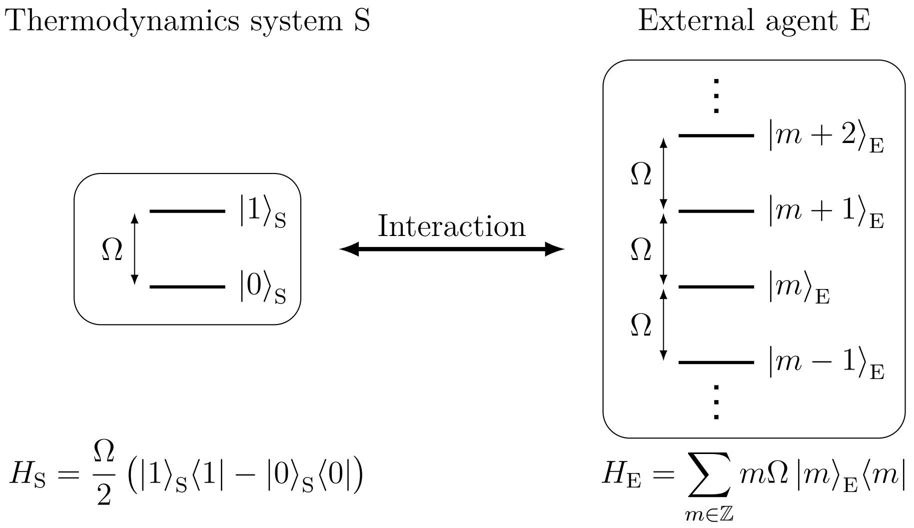

Figure 5.1: Illustration of the systems in the section 5.1. The operators H_S and H_E denote the Hamiltonians of the thermodynamic system S and the external agent E, respectively, and the parameter Ω denotes the level spacing.

tively (the figure 5.1):

$$H_S := \frac{\Omega}{2}\big(|1\rangle_S\langle 1| - |0\rangle_S\langle 0|\big), \tag{5.1}$$

$$H_E := \sum_{m\in\mathbb{Z}} h_m |m\rangle_E\langle m|, \tag{5.2}$$

where Ω is the level spacing and $h_m := m\Omega$ is the eigenvalues of H_E.

Let ρ_S and σ_E denote initial state of the thermodynamic system S and the external agent E. Because the thermodynamic system S is the two-level system, we can write the initial state ρ_S in the form

$$\rho_S := p|0\rangle_S\langle 0| + (1-p)|1\rangle_S\langle 1| + q|0\rangle_S\langle 1| + q^*|1\rangle_S\langle 0| \tag{5.3}$$

with $0 \le p \le 1$, $q \in \mathbb{C}$ and $|q|^2 \le p(1-p) \le 1/4$.

We assume that the time evolution of the total system is unitary one given by an unitary operator U_{SE} and conserves the total energy as in

$$[H_S + H_E, U_{SE}] = 0. \tag{5.4}$$

From energy conservation (5.4), we can write the unitary operator U_{SE} in the form

$$U_{SE} = \sum_{n,n'} K_{n,n'} \otimes |n\rangle_E\langle n'| \tag{5.5}$$

with

$$K_{n,n'} := \delta_{n,n'}\big(a_n|0\rangle_S\langle 0| + b_n|1\rangle_S\langle 1|\big) + \delta_{n-1,n'}c_n|0\rangle_S\langle 1| + \delta_{n+1,n'}d_n|1\rangle_S\langle 0| \tag{5.6}$$

for all integers n and n', where the coefficients a_n, b_n, c_n and d_n are complex numbers. Because U_{SE} is the unitary operator, we obtain $\sum_m K^\dagger_{m,n} K_{m,n'} = \delta_{n,n'} I_{\mathrm{S}}$, where I_{S} is an identity operator on the thermodynamic system S, and thereby obtain

$$|a_n|^2 + |d_{n-1}|^2 = 1, \tag{5.7a}$$

$$|b_n|^2 + |c_{n+1}|^2 = 1, \tag{5.7b}$$

$$a_n^* c_n + d_{n-1}^* b_{n-1} = 0 \tag{5.7c}$$

for all integers n. Then, the time-evolution map $\mathcal{K}$ of the thermodynamic system S is given by

$$\mathcal{K}(\rho_{\mathrm{S}}) := \mathrm{Tr}_{\mathrm{E}}\left[U_{\mathrm{SE}}(\rho_{\mathrm{S}} \otimes \sigma_{\mathrm{E}})U_{\mathrm{SE}}^\dagger\right] \tag{5.8}$$

$$= \sum_{n,n',n'' \in \mathbb{Z}} {}_{\mathrm{E}}\langle n' \,|\, \sigma_{\mathrm{E}} \,|\, n'' \rangle_{\mathrm{E}} K_{n,n'} \rho_{\mathrm{S}} K^\dagger_{n,n''}, \tag{5.9}$$

where Tr_{E} is partial trace over the external agent E.

For the time evolution of the thermodynamic system S to approximate to the unitary one, we choose the initial state σ_{E} and the unitary operator U_{SE} as

$$\sigma_{\mathrm{E}} = |\psi\rangle_{\mathrm{E}}\langle\psi|, \quad |\psi\rangle_{\mathrm{E}} := \frac{1}{\sqrt{M}} \sum_{m=1}^{M} |m\rangle_{\mathrm{E}}, \tag{5.10a}$$

$$U_{\mathrm{SE}} = \sum_{n,n'=0,1} |n\rangle_{\mathrm{S}}\langle n|U_{\mathrm{S}}|n'\rangle_{\mathrm{S}}\langle n'| \otimes W_{\mathrm{E}}^{n'-n} \tag{5.10b}$$

for an arbitrary unitary operator U_{S} on the thermodynamic system S, where M is a natural number and $W_{\mathrm{E}} := \sum_{m \in \mathbb{Z}} |m+1\rangle_{\mathrm{E}}\langle m|$ is the shift operator on the external agent E. Then, we can approximate the time-evolution map $\mathcal{K}$ of the equation (5.9) to the unitary evolution given by the unitary operator U_{S} when the natural number M in the equation (5.10a) becomes large enough [93, 96]:

$$\mathcal{K}(\rho_{\mathrm{S}}) \xrightarrow{M\to\infty} U_{\mathrm{S}} \rho_{\mathrm{S}} U_{\mathrm{S}}. \tag{5.11}$$

The coefficients a_n, b_n, c_n and d_n of the equation (5.6) become

$$a_n = {}_{\mathrm{S}}\langle 0 \,|\, U_{\mathrm{S}} \,|\, 0 \rangle_{\mathrm{S}} =: u_{0,0}, \tag{5.12a}$$

$$b_n = {}_{\mathrm{S}}\langle 1 \,|\, U_{\mathrm{S}} \,|\, 1 \rangle_{\mathrm{S}} =: u_{1,1}, \tag{5.12b}$$

$$c_n = {}_{\mathrm{S}}\langle 0 \,|\, U_{\mathrm{S}} \,|\, 1 \rangle_{\mathrm{S}} =: u_{0,1}, \tag{5.12c}$$

$$d_n = {}_{\mathrm{S}}\langle 1 \,|\, U_{\mathrm{S}} \,|\, 0 \rangle_{\mathrm{S}} =: u_{1,0} \tag{5.12d}$$

for all integers n.

First, we consider the variance of the energy loss of the thermodynamic system S. To calculate the variance of the energy loss, we define a single-shot energy loss by a difference of energy-measurement outcomes before and after the time evolution (5.9). In the time-dependent Hamiltonian approach, particularly quantum fluctuation theorems, this quantity is defined as the work extracted by the external agent (see the sections 3.3.1 or 4.1). From the time evolution (5.9) of the thermodynamic system S, the probability of the energy loss of the thermodynamic system

$$\upsilon_{k,l} := e_k - e_l \tag{5.13}$$

is given by

$$q_{k,l} := {}_{\mathrm{S}}\langle k \,|\, \rho_{\mathrm{S}} \,|\, k \rangle_{\mathrm{S}} \operatorname{Tr}\big[|l\rangle_{\mathrm{S}}\langle l|\mathcal{K}\big(|k\rangle_{\mathrm{S}}\langle k|\big)\big], \tag{5.14}$$

where $e_0 := -\Omega/2$ and $e_1 := \Omega/2$ are the eigenvalues of the Hamiltonian in the equation (5.1). Because the time evolution (5.9) satisfies the trace preserving, the average of $\upsilon_{k,l}$ is equal to the average energy loss of thermodynamic system S:

$$\langle \upsilon \rangle_{\mathrm{S}} := \sum_{k,l} \upsilon_{k,l} q_{k,l} = \operatorname{Tr}[\rho_{\mathrm{S}} H_{\mathrm{S}}] - \operatorname{Tr}[\mathcal{K}(\rho_{\mathrm{S}}) H_{\mathrm{S}}]. \tag{5.15}$$

We now define the variance of the energy loss of the thermodynamic system by

$$\mathrm{Var}_{\mathrm{S}}[\upsilon] := \big\langle \upsilon^2 \big\rangle_{\mathrm{S}} - \langle \upsilon \rangle_{\mathrm{S}}^2 . \tag{5.16}$$

Since $e_0 = -\Omega/2$ and $e_1 = \Omega/2$, the square of the energy loss $\upsilon_{k,l}^2$ is equal to zero or Ω^2. Therefore, we obtain $\big\langle \upsilon^2 \big\rangle_{\mathrm{S}} \le \Omega^2$. From $\langle \upsilon \rangle_{\mathrm{S}}^2 \ge 0$, we obtain an upper bundle on the variance $\mathrm{Var}_{\mathrm{S}}[\upsilon]$ in the from

$$\mathrm{Var}_{\mathrm{S}}[\upsilon] \le \Omega^2. \tag{5.17}$$

Note that this upper bound holds regardless of a form of the time evolution of the thermodynamic system S. Hence, the variance $\mathrm{Var}_{\mathrm{S}}[\upsilon]$ of the energy loss of the thermodynamic system S is always smaller than Ω^2 when the time evolution of the thermodynamic system S is approximated to the unitary one.

We next consider the variance of the energy obtained by the external agent E. By referring to the section 4.4, we define

$$w_j := h_j - \operatorname{Tr}_{\mathrm{E}}[\sigma_{\mathrm{E}} H_{\mathrm{E}}] \tag{5.18}$$

as the energy obtained by the external agent E and its probability is given by

$$\begin{aligned} p_j &:= \operatorname{Tr}\big[|j\rangle_{\mathrm{E}}\langle j| U_{\mathrm{SE}}(\rho_{\mathrm{S}} \otimes \sigma_{\mathrm{E}}) U_{\mathrm{SE}}^{\dagger}\big] && (5.19)\\ &= \sum_{n,n' \in \mathbb{Z}} {}_{\mathrm{E}}\langle n \,|\, \sigma_{\mathrm{E}} \,|\, n' \rangle_{\mathrm{E}} \operatorname{Tr}\big[K_{j,n'}^{\dagger} K_{j,n} \rho_{\mathrm{S}}\big], && (5.20) \end{aligned}$$

where Tr is trace over all systems. From the equations (5.4), the average of w_j is equal to the average energy loss of the thermodynamic system S of the equation (5.15):

$$\begin{aligned} \langle w \rangle_{\mathrm{E}} &:= \sum_{j \in \mathbb{Z}} w_j p_j && (5.21)\\ &= \operatorname{Tr}\big[H_{\mathrm{E}} U_{\mathrm{SE}}(\rho_{\mathrm{S}} \otimes \sigma_{\mathrm{E}}) U_{\mathrm{SE}}^{\dagger}\big] - \operatorname{Tr}_{\mathrm{E}}[\sigma_{\mathrm{E}} H_{\mathrm{E}}] && (5.22)\\ &= \operatorname{Tr}[(H_{\mathrm{S}} + H_{\mathrm{E}})(\rho_{\mathrm{S}} \otimes \sigma_{\mathrm{E}})] - \operatorname{Tr}\big[H_{\mathrm{S}} U_{\mathrm{SE}}(\rho_{\mathrm{S}} \otimes \sigma_{\mathrm{E}}) U_{\mathrm{SE}}^{\dagger}\big] - \operatorname{Tr}_{\mathrm{E}}[\sigma_{\mathrm{E}} H_{\mathrm{E}}] && (5.23)\\ &= \operatorname{Tr}[\rho_{\mathrm{S}} H_{\mathrm{S}}] - \operatorname{Tr}[\mathcal{K}(\rho_{\mathrm{S}}) H_{\mathrm{S}}] && (5.24)\\ &= \langle \upsilon \rangle_{\mathrm{S}} . && (5.25) \end{aligned}$$

We define the variance of the obtained energy w_j by

$$\begin{aligned} \mathrm{Var}_{\mathrm{E}}[w] &\coloneqq \left\langle w^2 \right\rangle_{\mathrm{E}} - \langle w \rangle_{\mathrm{E}}^2 && (5.26) \\ &= \left\langle h^2 \right\rangle_{\mathrm{E}} - \langle h \rangle_{\mathrm{E}}^2, && (5.27) \end{aligned}$$

where $\langle h \rangle$ and $\left\langle h^2 \right\rangle$ are the average and the means square of h_j, respectively, with respect to the probability p_j.

We now assume that the time evolution of the thermodynamic system S is approximated to the unitary one using the equations (5.10). Then, the probability p_j in the equation (5.20) reduces to

$$p_j = \frac{1}{M} \mathrm{Tr}\left[\tilde{K}_j^\dagger \tilde{K}_j \rho_{\mathrm{S}} \right] \tag{5.28}$$

with

$$\tilde{K}_j \coloneqq \sum_{m=1}^{M} K_{j,m} = \sum_{n,n'=0,1} \sum_{m=1}^{M} \delta_{j-n'+n,m} u_{n,n'} |n\rangle_{\mathrm{S}} \langle n'| \tag{5.29}$$

We can write $\langle h \rangle_{\mathrm{E}}$ and $\left\langle h^2 \right\rangle_{\mathrm{E}}$ in the forms

$$\begin{aligned} \langle h \rangle_{\mathrm{E}} &= \frac{\Omega}{M} \sum_j j \mathrm{Tr}\left[K_j^\dagger K_j \rho \right], && (5.30) \\ \left\langle h^2 \right\rangle_{\mathrm{E}} &= \frac{\Omega^2}{M} \sum_j j^2 \mathrm{Tr}\left[K_j^\dagger K_j \rho \right]. && (5.31) \end{aligned}$$

From the equation (5.29), we find

$$\tilde{K}_j = \begin{cases} u_{1,0} |1\rangle_{\mathrm{S}} \langle 0| & \text{for } j = 0 \\ U_{\mathrm{S}} - u_{0,1} |0\rangle_{\mathrm{S}} \langle 1| & \text{for } j = 1 \\ U_{\mathrm{S}} & \text{for } 2 \le j \le M-1 \\ U_{\mathrm{S}} - u_{1,0} |1\rangle_{\mathrm{S}} \langle 0| & \text{for } j = M \\ u_{0,1} |0\rangle_{\mathrm{S}} \langle 1| & \text{for } j = M+1 \\ 0 & \text{otherwise} \end{cases}, \tag{5.32}$$

and thereby obtain

$$\tilde{K}_j^\dagger \tilde{K}_j = \begin{cases} \left| u_{1,0} \right|^2 |0\rangle_{\mathrm{S}} \langle 0| & \text{for } j = 0 \\ I_{\mathrm{S}} - \left| u_{0,1} \right|^2 |1\rangle_{\mathrm{E}} \langle 1| + u_{0,1}^* u_{0,0} |1\rangle_{\mathrm{S}} \langle 0| + u_{0,1} u_{0,0}^* |0\rangle_{\mathrm{S}} \langle 1| & \text{for } j = 1 \\ I_{\mathrm{S}} & \text{for } 2 \le j \le M-1 \\ I_{\mathrm{S}} - \left| u_{1,0} \right|^2 |0\rangle_{\mathrm{E}} \langle 0| + u_{1,0}^* u_{1,1} |0\rangle_{\mathrm{S}} \langle 1| + u_{1,0} u_{1,1}^* |1\rangle_{\mathrm{S}} \langle 0| & \text{for } j = M \\ \left| u_{0,1} \right|^2 |1\rangle_{\mathrm{S}} \langle 1| & \text{for } j = M+1 \\ 0 & \text{otherwise} \end{cases}. \tag{5.33}$$

Using the relations (5.7) and (5.12), we obtain

$$\sum_j j\tilde{K}_j^\dagger \tilde{K}_j = \frac{M(M+1)}{2} I_\mathrm{S} - M\Big(|u_{1,0}|^2\, |0\rangle_\mathrm{E}\langle 0| - |u_{0,1}|^2\, |1\rangle_\mathrm{S}\langle 1|\Big) \\ + (M-1)\big(u_{1,0}^* u_{1,1} |0\rangle_\mathrm{S}\langle 1| + u_{1,0} u_{1,1}^* |1\rangle_\mathrm{S}\langle 0|\big), \quad (5.34)$$

$$\sum_j j^2 \tilde{K}_j^\dagger \tilde{K}_j = \frac{M(M+1)(2M+1)}{6} I_\mathrm{S} - M^2 |u_{1,0}|^2\, |0\rangle_\mathrm{E}\langle 0| + M(M+2)\, |u_{0,1}|^2\, |1\rangle_\mathrm{S}\langle 1| \\ + \big(M^2-1\big)\big(u_{1,0}^* u_{1,1} |0\rangle_\mathrm{S}\langle 1| + u_{1,0} u_{1,1}^* |1\rangle_\mathrm{S}\langle 0|\big). \quad (5.35)$$

Using the equation (5.3), the equations (5.30) and (5.31) are respectively given by

$$\frac{\langle h\rangle_\mathrm{E}}{\Omega} = \frac{(M+1)}{2} - |u_{1,0}|^2\, p + |u_{0,1}|^2\, (1-p) + 2\big(1-M^{-1}\big)\mathrm{Re}\big[u_{1,0}^* u_{1,1} q\big], \quad (5.36)$$

$$\frac{\langle h^2\rangle_\mathrm{E}}{\Omega^2} = \frac{(M+1)(2M+1)}{6} - M\, |u_{1,0}|^2\, p + (M+2)\, |u_{0,1}|^2\, (1-p) \\ + 2\big(M-M^{-1}\big)\mathrm{Re}\big[u_{1,0}^* u_{1,1} q\big]. \quad (5.37)$$

From the equation (5.18), we can obtain

$$\langle h\rangle_\mathrm{E} = \langle w\rangle + \mathrm{Tr}_\mathrm{E}[\sigma_\mathrm{E} H_\mathrm{E}] = \langle w\rangle + \frac{M+1}{2}\Omega. \quad (5.38)$$

Comparing the above equation and (5.36), we obtain

$$\langle w\rangle_\mathrm{E} = \Omega\Big[|u_{0,1}|^2\, (1-p) - |u_{1,0}|^2\, p + 2\big(1-M^{-1}\big)\mathrm{Re}\big[u_{1,0}^* u_{1,1} q\big]\Big], \quad (5.39)$$

and thereby obtain

$$\big\langle h^2\big\rangle_\mathrm{E} = \frac{(M+1)(2M+1)}{6}\Omega + (M+1)\Omega\, \langle w\rangle_\mathrm{E} + \Omega^2\Big(|u_{1,0}|^2\, p + |u_{0,1}|^2\, (1-p)\Big). \quad (5.40)$$

Inserting the equations (5.38) and (5.40) into the equation (5.27), we obtain

$$\mathrm{Var}_\mathrm{E}[w] = \frac{M^2-1}{12}\Omega^2 - \langle w\rangle_\mathrm{E}^2 + \Omega^2\Big(|u_{1,0}|^2\, p + |u_{0,1}|^2\, (1-p)\Big). \quad (5.41)$$

Because $\langle w\rangle_\mathrm{E} = \Omega\, O(1)$ as $M \to \infty$ from the equation (5.39), the variance $\mathrm{Var}_\mathrm{E}[w]$ becomes

$$\mathrm{Var}_\mathrm{E}[w] = \Omega^2 O\big(M^2\big) \quad (M \to \infty). \quad (5.42)$$

Hence, the variance of the energy obtained by the external agent E diverges when the time evolution of the thermodynamic system S is approximated to the unitary one. This behavior is clearly difference from the variance of the energy loss of the thermodynamic system S of the equation (5.17).

The above demonstration proves a problem of the time-dependent Hamiltonian approach, which employ a unitary evolution of the thermodynamic system and regard its energy loss as the work. In particularly, because the energy obtained by the external agent is the actual work, we can recognize that the quantum version of the work fluctuation relations derived in the conventional approach (see the sections 3.3.1 and 3.3.2) do not contain relevant information about the fluctuation of the actual work. In order to resolve this problem, we derive in the section 5.2 the quantum Jarzynski equality using the new formulation of the chapter 4.

Incidentally, we show that we cannot approximate the time evolution to a unitary one in the case $M = 1$. To show it, we calculate the quantity

$$\min_{U^\dagger U = I_\mathrm{S}} d\big(\mathcal{K}(\rho_\mathrm{S}), U\rho_\mathrm{S}U^\dagger\big), \tag{5.43}$$

where $d(A, B) := (1/2)\mathrm{Tr}\,|A - B|$ is the trace distance [24, 108] of operators A and B. For $M = 1$, the initial state of the external agent E is a pure energy eigenstate. We now choose a energy eigenstate of a fixed energy level n_0 as the initial state σ_E, namely, $\sigma_\mathrm{E} = |n_0\rangle_\mathrm{E}\langle n_0|$. Then, the time-evolution map (5.9) reduces to

$$\begin{aligned}\mathcal{K}(\rho_\mathrm{S}) &= \sum_{n\in\mathbb{Z}} K_{n,n_0}\rho_\mathrm{S}K^\dagger_{n,n_0}\\ &= \Big[|a_{n_0}|^2\,p + |c_{n_0+1}|^2\,(1-p)\Big]|0\rangle_\mathrm{S}\langle 0| + \Big[|b_{n_0}|^2\,(1-p) + |d_{n_0-1}|^2\,p\Big]|1\rangle_\mathrm{S}\langle 1|\\ &\qquad + a_{n_0}b^*_{n_0}|0\rangle_\mathrm{S}\langle 1| + a^*_{n_0}b_{n_0}|1\rangle_\mathrm{S}\langle 0|.\end{aligned} \tag{5.44}$$

From the equations (5.7) and (5.24), we obtain

$$\langle w\rangle_\mathrm{E} = \Omega[x(1-p) + yp] \tag{5.45}$$

with $x := |c_{n_0+1}|^2$ and $y := |d_{n_0-1}|^2$.

Let us calculate the equation (5.43). Because the state ρ_S is a positive semi-definite operator, we obtain its eigenvalues $\lambda_\pm := (1/2) \pm R$ with

$$R := \sqrt{\left(p - \frac{1}{2}\right)^2 + |q|^2} \tag{5.46}$$

and define $|\phi_\pm\rangle$ as normalized eigenstates of $\lambda_\pm$, respectively. Then, we obtain

$$\rho_\mathrm{S} = \frac{1}{2}I_\mathrm{S} + R\big(|\phi_+\rangle_\mathrm{S}\langle\phi_+| - |\phi_-\rangle_\mathrm{S}\langle\phi_-|\big). \tag{5.47}$$

Similar to the state ρ, eigenvalues of the state $\mathcal{K}(\rho_\mathrm{S})$ are given by $\lambda'_\pm := (1/2) \pm R'$ with

$$R' := \sqrt{\left((1-x-y)p + x - \frac{1}{2}\right)^2 + (1-x)(1-y)\,|q|^2}, \tag{5.48}$$

and we define $|\phi'_\pm\rangle$ as normalized eigenstates of $\lambda'_\pm$, respectively. We obtain

$$\mathcal{K}(\rho_\mathrm{S}) = \frac{1}{2}I_\mathrm{S} + R\big(|\phi'_+\rangle_\mathrm{S}\langle\phi'_+| - |\phi'_-\rangle_\mathrm{S}\langle\phi'_-|\big). \tag{5.49}$$

Combining the equations (5.47) and (5.49), we obtain

$$\begin{aligned}&\mathcal{K}(\rho_\mathrm{S}) - U\rho_\mathrm{S}U^\dagger \\ &\qquad = R'\big(|\phi'_+\rangle_\mathrm{S}\langle\phi'_+| - |\phi'_-\rangle_\mathrm{S}\langle\phi'_-|\big) - R\big(U|\phi_+\rangle_\mathrm{S}\langle\phi_+|U^\dagger - U|\phi_-\rangle_\mathrm{S}\langle\phi_-|U^\dagger\big),\end{aligned} \tag{5.50}$$

where U is an arbitrary unitary operator.

The arbitrary unitary operator U can be given by

$$U = e^{i\phi}\big(\alpha|\phi'_+\rangle_\mathrm{S}\langle\phi_+| - \beta^*|\phi'_+\rangle_\mathrm{S}\langle\phi_-| + \beta|\phi'_-\rangle_\mathrm{S}\langle\phi_+| + \alpha^*|\phi'_-\rangle_\mathrm{S}\langle\phi_-|\big), \tag{5.51}$$

where α and β are complex parameters satisfying $|\alpha|^2 + |\beta|^2 = 1$ and θ is a real parameter. Using above representation, we obtain

$$\begin{aligned}&\mathcal{K}(\rho_\mathrm{S}) - U\rho_\mathrm{S}U^\dagger \\ &\qquad = \big[R' - R\big(|\alpha|^2 - |\beta|^2\big)\big]|\phi'_+\rangle_\mathrm{S}\langle\phi'_+| - \big[R' + R\big(|\beta|^2 - |\alpha|^2\big)\big]|\phi'_-\rangle_\mathrm{S}\langle\phi'_-| \\ &\qquad\qquad - 2\alpha\beta R|\phi'_+\rangle_\mathrm{S}\langle\phi'_-| - 2\alpha^*\beta^* R|\phi'_-\rangle_\mathrm{S}\langle\phi'_+|.\end{aligned} \tag{5.52}$$

From $|\alpha|^2 + |\beta|^2 = 1$, the eigenvalues of $\mathcal{K}(\rho_\mathrm{S}) - U\rho_\mathrm{S}U^\dagger$ are given by $\pm\sqrt{R'^2 + R^2 - 2|\alpha|^2|\beta|^2 RR'}$, and we thereby obtain

$$\frac{1}{2}\mathrm{Tr}\,|\mathcal{K}(\rho_\mathrm{S}) - U\rho_\mathrm{S}U^\dagger| = \sqrt{R'^2 + R^2 - 2|\alpha|^2|\beta|^2 RR'}. \tag{5.53}$$

The equation (5.43) is minimization of the above equation with respect to the unitary operator U, namely, the parameters α and β. We therefore obtain

$$\min_{U^\dagger U = I_\mathrm{S}} d\big(\mathcal{K}(\rho_\mathrm{S}), U\rho_\mathrm{S}U^\dagger\big) = \min_{|\alpha|^2+|\beta|^2=1} \sqrt{R'^2 + R^2 - 2|\alpha|^2|\beta|^2 RR'} \tag{5.54}$$

$$= \sqrt{R'^2 + R^2}. \tag{5.55}$$

In case of $x = y = 0$, the quantity R' reduces to R and the distance of the equation (5.55) is then equal to zero. This means that the time evolution can be approximated to the unitary one. However, the average work of the equation (5.45) is always equal to zero. For that reason, we have to consider cases other then $x = y = 0$. If we choose the initial state of the thermodynamic system S as $p = 1/2$ and $|q| = 0$, the distance of the equation (5.55) is not equal to zero without $x = y = 0$ (the figure 5.2(a)). Similarly, if we choose the initial state as $p = |q| = 1/2$, the distance of the equation (5.55) is not equal to zero for $x = y \neq 0$ (the figure 5.2(b)). Therefore, we cannot approximate the time evolution of the thermodynamic system S to the unitary one in the case $M = 1$.

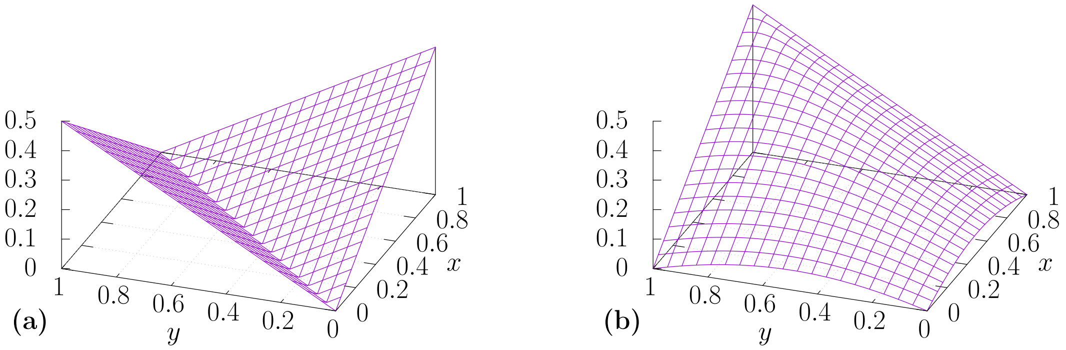

Figure 5.2: Plots of the equation (5.55) taking the parameters (a) $(p, |q|) = (1/2, 0)$ and (b) $(1/2, 1/2)$.

5.2 Jarzynski equality

From the previous section, we showed a problem of the quantum version of the Jarzynski equality derived the conventional approach [23, 25, 48, 66], which assumes a unitary evolution of a thermodynamic system and regard the energy loss of the thermodynamic system as the work. To resolve this problem, we here derive the quantum version of the Jarzynski equality using the new formulation of work extraction in the chapter 4.

5.2.1 Cyclic process

We first consider the case of a cyclic process, in which the final Hamiltonian is equal to the initial one. We assume that a thermodynamic system is performed the cyclic process by an external agent and the external agent obtain the energy from the thermodynamic system as the work.

Let H_{S} and H_{E} denote the initial Hamiltonian of the thermodynamic system S and the external agent E. The eigenvalue decompositions of H_{S} and H_{E} are denoted by

$$H_{\mathrm{S}} := \sum_x h_x |h_x\rangle_{\mathrm{S}}\langle h_x|, \tag{5.56}$$

$$H_{\mathrm{E}} := \sum_i e_i |e_i\rangle_{\mathrm{E}}\langle e_i|, \tag{5.57}$$

where h_x and e_i are the eigenvalues of H_{S} and H_{E} (the figure 5.3(a)).

Referring to fully quantum model of work extraction in the section 4.4, we assume that the cyclic process of the total system is given by the unitary evolution given by a unitary operator U_{SE} which satisfies the energy conservation

$$[H_{\mathrm{S}} + H_{\mathrm{E}}, U_{\mathrm{SE}}] = 0. \tag{5.58}$$

We further assume that the initial state of the thermodynamic system S and the external agent E are given by the canonical distribution at an inverse temperature β and a pure

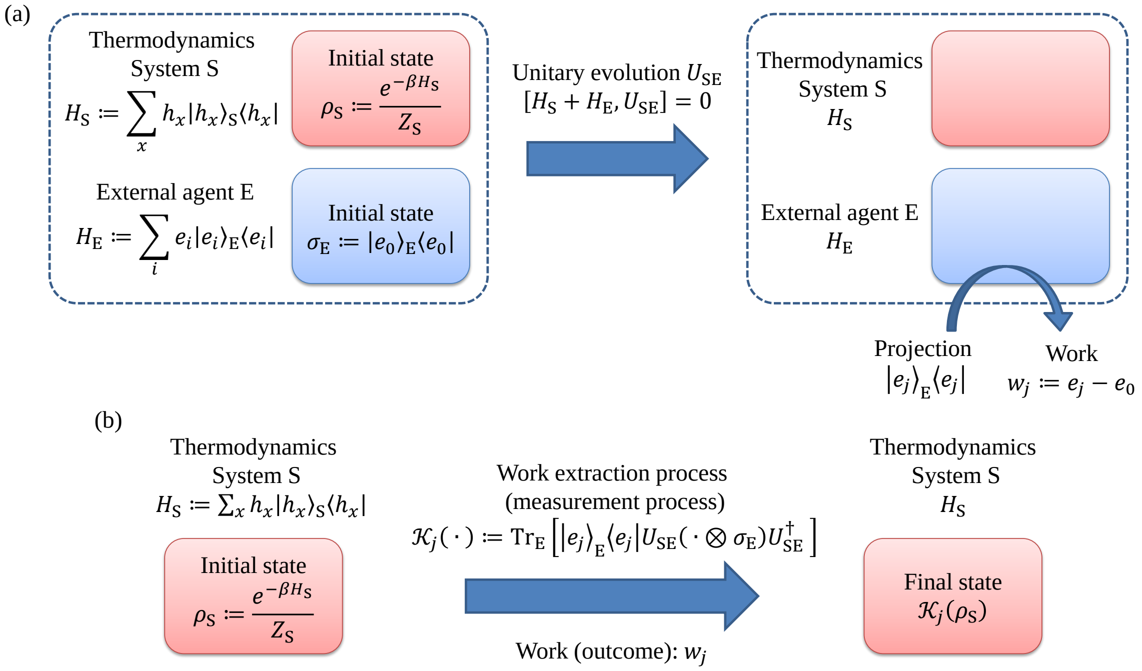

Figure 5.3: (a) Illustration of the cyclic process of the thermodynamic system S performed by the external agent E. The cyclic process means that the final Hamiltonian is equal to the initial one. We now represent the cyclic process by the unitary evolution U_{SE} of the total system. After the cyclic process, we measure the energy of the external agent E using the projection $|e_j\rangle_E\langle e_j|$ and define $w_j := e_j - e_0$ as the work extracted by the external agent E. (b) Illustration of the cyclic process of the thermodynamic system S after trace over the external agent E. The cyclic process reduces to the work extraction process $\mathcal{K}_j$ defined by the measurement process (5.65) and the corresponding work is w_j. The work extraction process $\mathcal{K}_j$ satisfies the strong energy conservation of the equation (5.66).

energy eigenstate of energy e_0, respectively:

$$\rho_S := \sum_x \frac{e^{-\beta h_x}}{Z_S} |h_x\rangle_S\langle h_x|, \tag{5.59}$$

$$\sigma_S := |e_0\rangle_E\langle e_0| \tag{5.60}$$

$$\tag{5.61}$$

with $Z_S := \mathrm{Tr}\left[e^{-\beta H_S}\right]$.

According to the fully quantum model of work extraction in the section 4.4, we consider the following process (see the figure 5.3(a)):

1. We set the initial states of the thermodynamic system S and the external agent E given by the equations (5.59) and (5.60): the initial state of the total system is given by

$$\rho_S \otimes \sigma_E. \tag{5.62}$$

2. We evolves the total system according to the unitary operator U_{SE}: the state of the total system becomes
$$U_{\mathrm{SE}}(\rho_{\mathrm{S}} \otimes \sigma_{\mathrm{E}})U_{\mathrm{SE}}^{\dagger}. \tag{5.63}$$
The key point is to consider the unitary evolution of the total system, not of the thermodynamic system S.
3. To know the amount of the extracted work, we finally measure the energy of the external agent E using the projection $|e_j\rangle_{\mathrm{E}}\langle e_j|$ and define
$$w_j := e_j - e_0 \tag{5.64}$$
as the work extracted by the external agent E. It is essential that at this point the "work" w_j is not a fixed value but given probabilistically.

In the above process, we obtain the work extraction process of the specific extracted work w_j in the form

$$\mathcal{K}_j(\rho_{\mathrm{S}}) := \mathrm{Tr}_{\mathrm{E}}\Big[|e_j\rangle_{\mathrm{E}}\langle e_j|U_{\mathrm{SE}}(\rho_{\mathrm{S}} \otimes \sigma_{\mathrm{E}})U_{\mathrm{SE}}^{\dagger}\Big], \tag{5.65}$$

where Tr_{E} is partial trace over the external agent E (the figure 5.3(b)). Because the unitary evolution of the total system satisfies the energy conservation (5.58) and the initial state of the external agent E is the pure energy eigenstate (5.60), the work extraction process $\mathcal{K}_j$ satisfies the strong energy conservation of the equation (4.6) in the section 4.3, namely, satisfies
$$\mathcal{K}_j\big(|h_x\rangle_{\mathrm{S}}\langle h_x|\big) = P_{h_x-w_j}\mathcal{K}_j\big(|h_x\rangle_{\mathrm{S}}\langle h_x|\big)P_{h_x-w_j} \tag{5.66}$$
for all j, x, where $P_h := \sum_y \delta_{h,h_y}|h_y\rangle_{\mathrm{S}}\langle h_y|$ (see the section 4.4).

We then define the probability distribution of a random variable W with respect to the extracted work by
$$P(W) := \sum_j \delta\big(W - w_j\big)\mathrm{Tr}\big[\mathcal{K}_j(\rho_{\mathrm{S}})\big], \tag{5.67}$$

where $\delta(x)$ and Tr are the delta function and the trace over all system, respectively. Because $\mathcal{K}_j$ is a linear map and $\sum_y |h_y\rangle_{\mathrm{S}}\langle h_y| = I_{\mathrm{S}}$, where I_{S} is the identity operator on the thermodynamic system S, we obtain

$$P(W) = \sum_{j,x,y} \delta\big(W - w_j\big)\frac{e^{-\beta h_x}}{Z_{\mathrm{S}}}\mathrm{Tr}\Big[|h_y\rangle_{\mathrm{S}}\langle h_y|\mathcal{K}_j\big(|h_x\rangle_{\mathrm{S}}\langle h_x|\big)\Big]. \tag{5.68}$$

From the strong energy conservation of the equation (5.66), the extracted work w_j must be equal to the energy loss $h_x - h_y$ of the thermodynamic system S after the work extraction process $\mathcal{K}_j$. Hence, we find

$$\begin{aligned} P(W) &= \sum_{j,x,y} \delta\big(W - w_j\big)\frac{e^{-\beta(w_j+h_y)}}{Z_{\mathrm{S}}}\mathrm{Tr}\Big[|h_y\rangle_{\mathrm{S}}\langle h_y|\mathcal{K}_j\big(|h_x\rangle_{\mathrm{S}}\langle h_x|\big)\Big] && (5.69)\\ &= e^{-\beta W}\sum_j \delta\big(W - w_j\big)\mathrm{Tr}\big[\rho_{\mathrm{S}}\mathcal{K}_j(I_{\mathrm{S}})\big]. && (5.70) \end{aligned}$$

Let us denote the average with respect to the probability distribution $P(W)$ by

$$\langle f(W)\rangle := \int dW\, f(W)\, P(W), \tag{5.71}$$

where $f(W)$ is a function of the random variable W. Using the equation (5.70), we then obtain the Jarzynski equality under the cyclic process in the form

$$\left\langle e^{\beta W}\right\rangle = \gamma \tag{5.72}$$

with

$$\gamma := \mathrm{Tr}[\rho_{\mathrm{S}}\mathcal{K}(I_{\mathrm{S}})], \tag{5.73}$$

where $\mathcal{K}$ is the time-evolution map of the thermodynamic system S defined by

$$\mathcal{K}(\rho_{\mathrm{S}}) := \sum_j \mathcal{K}_j(\rho_{\mathrm{S}}) = \mathrm{Tr}_{\mathrm{E}}\left[U_{\mathrm{SE}}(\rho_{\mathrm{S}} \otimes \sigma_{\mathrm{E}})U_{\mathrm{SE}}^{\dagger}\right]. \tag{5.74}$$

Note that we did not use the detail of the external agent E to derive the equation (5.72) but the strong energy conservation (5.66) of the work extraction process $\mathcal{K}_j$ of the thermodynamic system S.

Applying Jensen's inequality $\left\langle e^{f}\right\rangle \geq e^{\langle f\rangle}$ to the equation (5.72), we obtain the second law of thermodynamics under the measurement-based work extraction in the form

$$\langle W\rangle \leq \beta^{-1}\log\gamma. \tag{5.75}$$

Let us assume that the time evolution of the thermodynamics system S is a "natural" thermodynamic process. The "natural" thermodynamic process means the work extraction process which does not operator a feedback operation and satisfies the first and second laws of thermodynamics for an arbitrary initial state. From the strong energy conservation of the equation (5.66), the work extraction process $\mathcal{K}_j$ clearly satisfies the first law of thermodynamics for an arbitrary initial state. On the other hand, to satisfy the second law for an arbitrary initial state, we append the following condition to the time-evolution map $\mathcal{K}$:

$$S(\rho) \leq S(\mathcal{K}(\rho)) \tag{5.76}$$

for an arbitrary initial state ρ of the thermodynamic system S, where $S(\rho) := -\mathrm{Tr}\left[\rho\log\rho\right]$ is the von Neumann entropy. As a necessary and sufficient condition of the equation (5.76) for an arbitrary initial state, the time-evolution map $\mathcal{K}$ must be a unital map [51]:

$$\mathcal{K}(I_{\mathrm{S}}) = I_{\mathrm{S}}. \tag{5.77}$$

Inserting the equation (5.77) into the equation (5.73), we obtain $\gamma = 1$ and thereby obtain

$$\left\langle e^{\beta W}\right\rangle = 1, \tag{5.78}$$

$$\langle W\rangle \leq 0. \tag{5.79}$$

Hence, we can obtain the same form as the quantum Jarzynski equality derived the conventional approach [23, 25, 48, 66] under the cyclic process when the work extraction process is a "natural" thermodynamic process.

The difference of the right-hand side of the Jarzynski equality from unity is known for feedback processes [62, 71, 74, 106] and/or absolutely irreversible process [100, 106]. The difference is represented as an feedback efficiency [62] for the feedback process, on the other hand, comes from a probability of the singular part [100] for the absolutely irreversible. In case of this section, we do not apply the absolutely irreversible to the equation (5.72), because the initial state (5.59) of the thermodynamic system S is the canonical distribution and thereby does not have the singular part. On the other hand, because the time-evolution map $\mathcal{K}$ includes the feedback process, we can regard the coefficient γ of the equation (5.73) as the feedback efficiency.

We stress that the quantum Jarzynski equation of this derivation is essentially different from those of the conventional derivation [23, 25, 48, 66] in the section 3.3.1. The conventional derivation of the quantum Jarzynski equality defined the measured value of the energy loss of the unitary-evolving thermodynamic system as the random variable W, and thereby did not appropriately contain information about the fluctuation of the energy obtained by the external agent. As we have shown in the section 5.1, the variance of the work W in the conventional derivation is completely different from that of the energy obtained by the external agent, which is the actual work that we can use, under the approximation of the unitary evolution of the thermodynamic system. Therefore, the quantum Jarzynski equality of the conventional derivation does not give relevant information about the fluctuation of the actual work.

On the other hand, the present derivation of the quantum Jarzynski equality is different in this point. Because we now employ the unitary evolution of the total system satisfying the energy conservation of the equation (5.58), we also define the measured value of the energy loss of the thermodynamic system as a random variable W, but it is equal to the measured value of the energy obtained by the external agent. Therefore, the present derivation correctly contains the information about the fluctuation of the actual work.

5.2.2 Non-cyclic process

We next consider the case of a non-cyclic process, extending the case of the cyclic process in the section 5.2.1 using a control system in the section 4.2. For a non-cyclic process, the Hamiltonian of a system of a driven system is different between the initial and final ones. To apply the derivation for the cyclic process to the non-cyclic one, we divide the thermodynamic system S into two subsystem [89, 93, 105, 110, 117]. One of the subsystem is an internal system I which is a working substance, such as a gas. The other subsystem is a control system C which controls the Hamiltonian of the internal system I as piston (the figure 5.4). We consider the work extracted from the internal system I.

Referring the section 4.2, let $\{ |\lambda\rangle_{\mathrm{C}} \}_{\lambda}$ denotes an orthonormal basis of the control system C corresponding to the value of the control parameter λ. We assume the initial Hamilto-

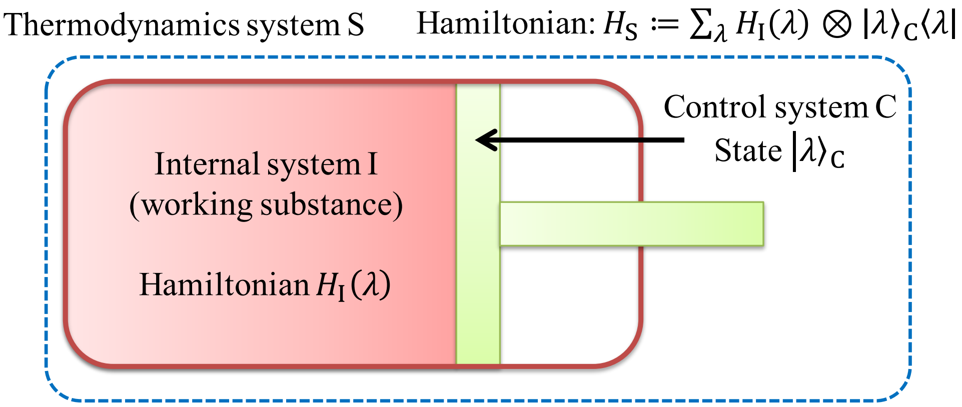

Figure 5.4: To apply the formalism for the cyclic process of the section 5.2.1 to the non-cyclic one, we divide the thermodynamic system S into two subsystems, namely an internal system I and a control system C (see the section 4.2).

nian (5.56) of the thermodynamic system S in the form

$$\begin{aligned} H_\mathrm{S} &:= \sum_\lambda H_\mathrm{I}(\lambda) \otimes |\lambda\rangle_\mathrm{C}\langle\lambda| \\ &= \sum_\lambda \sum_{x(\lambda)} h_{x(\lambda)} \left|h_{x(\lambda)}, \lambda\right\rangle_\mathrm{IC}\left\langle h_{x(\lambda)}, \lambda\right|, \end{aligned} \tag{5.80}$$

where $H_\mathrm{I}(\lambda)$ is the Hamiltonian of the internal system I, whose eigenstate and corresponding eigenvalue are denoted as $\left|h_{x(\lambda)}\right\rangle_\mathrm{I}$ and $h_{x(\lambda)}$, respectively; and $\left|h_{x(\lambda)}, \lambda\right\rangle_\mathrm{IC}$ denotes $\left|h_{x(\lambda)}\right\rangle_\mathrm{I} \otimes |\lambda\rangle_\mathrm{C}$. We change the control parameter λ, making the non-cyclic process. Note that the index $x(\lambda)$ depends on the control parameter λ, because the set of the eigenvalues of the Hamiltonian $H_\mathrm{I}(\lambda)$ depends on the control one λ. From the strong energy conservation (5.66) of the work extraction process $\mathcal{K}_j$, the energy of the internal system I changes from $h_{x(\lambda)}$ to $h_{x(\lambda)} - w_j$ after the work extraction process $\mathcal{K}_j$ of the specific extracted work w_j.

To start the internal system I from the equilibrium with a fixed parameter λ_i, we replace the initial state (5.59) of the thermodynamic system S by the canonical distribution of the internal system I with a pure state $|\lambda_\mathrm{i}\rangle_\mathrm{C}$ of the control system C (the figure 5.5):

$$\begin{aligned} \rho_\mathrm{S}(\lambda_\mathrm{i}) &:= \sum_{x(\lambda_\mathrm{i})} \frac{e^{-\beta h_{x(\lambda_\mathrm{i})}}}{Z_\mathrm{I}(\lambda_\mathrm{i})} \left|h_{x(\lambda_\mathrm{i})}, \lambda_\mathrm{i}\right\rangle_\mathrm{IC}\left\langle h_{x(\lambda_\mathrm{i})}, \lambda_\mathrm{i}\right| \\ &= \rho_\mathrm{I}(\lambda_\mathrm{i}) \otimes |\lambda_\mathrm{i}\rangle_\mathrm{C}\langle\lambda_\mathrm{i}| \end{aligned} \tag{5.81}$$

with $Z_\mathrm{I}(\lambda) := \mathrm{Tr}\left[e^{-\beta H_\mathrm{I}(\lambda)}\right]$ and $\rho_\mathrm{I}(\lambda) := e^{-\beta H_\mathrm{I}(\lambda)}/Z_\mathrm{I}(\lambda)$. The Helmholtz free energy of the internal system I for a specific parameter λ is given by

$$F_\mathrm{I}(\lambda) := -\beta^{-1} \log Z_\mathrm{I}(\lambda). \tag{5.82}$$

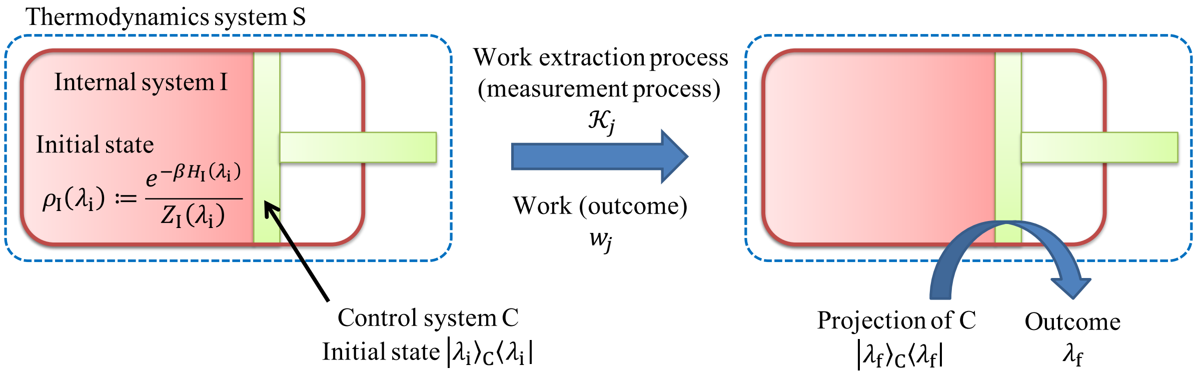

Figure 5.5: Illustration of the non-cyclic process of the thermodynamics system S. To apply the formalism for the cyclic process of the section 5.2.1 to the non-cyclic process using the division of the thermodynamic system S, we replace the initial state of the thermodynamic system S by the canonical distribution of the internal system I with a pure state $|\lambda_\mathrm{i}\rangle_\mathrm{C}$ of the control system C. The work extraction process $\mathcal{K}_j$ satisfies the strong energy conservation of the equation (5.66) in the section 5.2.1, and the extracted work is denoted by w_j. After the work extraction, we observe the control system C using the projection $|\lambda_\mathrm{f}\rangle_\mathrm{C}\langle\lambda_\mathrm{f}|$ to know the destination of the non-cyclic process.

We then define the probability distribution of the random variable W with respect to the extracted work during the process in which the state of the control system C changes from $|\lambda_\mathrm{i}\rangle_\mathrm{C}$ to $|\lambda_\mathrm{f}\rangle_\mathrm{C}$ as

$$P_{\lambda_\mathrm{i}\to\lambda_\mathrm{f}}(W) := \sum_j \frac{\delta\big(W - w_j\big)}{p_{\lambda_\mathrm{i}\to\lambda_\mathrm{f}}} \mathrm{Tr}\Big[|\lambda_\mathrm{f}\rangle_\mathrm{C}\langle\lambda_\mathrm{f}|\mathcal{K}_j\big(\rho_\mathrm{I}(\lambda_\mathrm{i}) \otimes |\lambda_\mathrm{i}\rangle_\mathrm{C}\langle\lambda_\mathrm{i}|\big)\Big], \tag{5.83}$$

where

$$p_{\lambda_\mathrm{i}\to\lambda_\mathrm{f}} := \mathrm{Tr}\Big[|\lambda_\mathrm{f}\rangle_\mathrm{C}\langle\lambda_\mathrm{f}|\mathcal{K}\big(\rho_\mathrm{I}(\lambda_\mathrm{i}) \otimes |\lambda_\mathrm{i}\rangle_\mathrm{C}\langle\lambda_\mathrm{i}|\big)\Big] \tag{5.84}$$

is the transition probability that the control parameter changes from λ_i to λ_f (see the figure 5.5). In the same way as in the equation (5.70) of the section 5.2.1, we obtain

$$\begin{aligned} P_{\lambda_\mathrm{i}\to\lambda_\mathrm{f}}(W) &= e^{-\beta(W+\Delta F_\mathrm{I}(\lambda_\mathrm{i},\lambda_\mathrm{f}))} \\ &\quad\times \sum_j \frac{\delta\big(W - w_j\big)}{p_{\lambda_\mathrm{i}\to\lambda_\mathrm{f}}} \mathrm{Tr}\Big[\rho_\mathrm{I}(\lambda_\mathrm{f}) \otimes |\lambda_\mathrm{f}\rangle_\mathrm{C}\langle\lambda_\mathrm{f}|\mathcal{K}_j\big(I_\mathrm{I}(\lambda_\mathrm{i}) \otimes |\lambda_\mathrm{i}\rangle_\mathrm{C}\langle\lambda_\mathrm{i}|\big)\Big], \end{aligned} \tag{5.85}$$

where $\Delta F_\mathrm{I}(\lambda_\mathrm{i}, \lambda_\mathrm{f}) := F_\mathrm{I}(\lambda_\mathrm{f}) - F_\mathrm{I}(\lambda_\mathrm{i})$ is the difference of the Helmholtz free energy of the internal system I and $I_\mathrm{I}(\lambda) := \sum_{x(\lambda)} |h_{x(\lambda)}\rangle_\mathrm{I}\langle h_{x(\lambda)}|$ is the identity operator of the internal system I with fixed control parameter λ.

Modifying the average (5.71) with respect to the probability distribution $P(W)$ to

$$\langle f(W)\rangle_{\lambda_\mathrm{i}\to\lambda_\mathrm{f}} := \int dW\, f(W)\, P_{\lambda_\mathrm{i}\to\lambda_\mathrm{f}}(W), \tag{5.86}$$

we therefore obtain the quantum Jarzynski equality under a non-cyclic process in the form

$$\left\langle e^{\beta W}\right\rangle_{\lambda_\mathrm{i}\to\lambda_\mathrm{f}} = \gamma_{\lambda_\mathrm{i}\to\lambda_\mathrm{f}} e^{-\beta\Delta F_\mathrm{I}(\lambda_\mathrm{i},\lambda_\mathrm{f})} \tag{5.87}$$

with

$$\gamma_{\lambda_\mathrm{i}\to\lambda_\mathrm{f}} := \frac{p_{\lambda_\mathrm{i}\to\lambda_\mathrm{f}}}{q_{\lambda_\mathrm{f}\to\lambda_\mathrm{i}}}, \tag{5.88}$$

$$q_{\lambda_\mathrm{f}\to\lambda_\mathrm{i}} := \mathrm{Tr}\Big[\rho_\mathrm{I}(\lambda_\mathrm{i})\otimes|\lambda_\mathrm{f}\rangle_\mathrm{C}\langle\lambda_\mathrm{f}|\mathcal{K}\big(I_\mathrm{I}(\lambda_\mathrm{i})\otimes|\lambda_\mathrm{i}\rangle_\mathrm{C}\langle\lambda_\mathrm{i}|\big)\Big]. \tag{5.89}$$

Note that we observe the initial and final states of the control system C, not its intermediate state. During the dynamics between these states, we cannot tell the path of the change of the control parameter, such as the position of a piston, nor can we tell the motion of the internal system I. It is in contrast with the fact that the motion of the system is fully determined by a given path of a parameter in the conventional derivation of the quantum Jarzynski equality [23, 25, 48, 66].

We now argue that the coefficient $\gamma_{\lambda_\mathrm{i}\to\lambda_\mathrm{f}}$ is not necessarily unity for a unital map as γ of the equation (5.73) was for the cyclic process. When the time-evolution map $\mathcal{K}$ is unital, namely the "natural" thermodynamic process defined in the section 5.2.1, the coefficient $\gamma_{\lambda_\mathrm{i}\to\lambda_\mathrm{f}}$ gives the ratio of the forward and backward transition probabilities. When the time-evolution map $\mathcal{K}$ is unital, trace preserving and completely positive, so is its adjoint $\mathcal{K}^\dagger$. In other words, the adjoint map $\mathcal{K}^\dagger$ is regarded as another time evolution. Therefore, the equation (5.89) gives the backward transition probability that the control parameter changes from λ_f to λ_i:

$$q_{\lambda_\mathrm{f}\to\lambda_\mathrm{i}} = \mathrm{Tr}\Big[|\lambda_\mathrm{i}\rangle_\mathrm{C}\langle\lambda_\mathrm{i}|\mathcal{K}^\dagger\big(\rho_\mathrm{I}(\lambda_\mathrm{f})\otimes|\lambda_\mathrm{f}\rangle_\mathrm{C}\langle\lambda_\mathrm{f}|\big)\Big]. \tag{5.90}$$

As can be seen from the calculation of a simple model in the section 5.3, the backward transition probability (5.90) is not necessarily equal to the forward one (5.84). Hence, the coefficient $\gamma_{\lambda_\mathrm{i}\to\lambda_\mathrm{f}}$ is not necessarily unity for the unital map.

When the time-evolution map $\mathcal{K}$ is not unital, incidentally, we cannot regard the equation (5.89) as a transition probability. Because the adjoint $\mathcal{K}^\dagger$ of a non-unital map $\mathcal{K}$ does not satisfy trace preserving, the sum of the equation (5.89) over λ_i is not unity:

$$\sum_{\lambda_\mathrm{i}} q_{\lambda_\mathrm{f}\to\lambda_\mathrm{i}} = \mathrm{Tr}\Big[\rho_\mathrm{I}(\lambda_\mathrm{i})\otimes|\lambda_\mathrm{f}\rangle_\mathrm{C}\langle\lambda_\mathrm{f}|\mathcal{K}(I_\mathrm{S}(\lambda_\mathrm{i}))\Big] \tag{5.91}$$

$$= \mathrm{Tr}\Big[\mathcal{K}\big(\rho_\mathrm{I}(\lambda_\mathrm{i})\otimes|\lambda_\mathrm{f}\rangle_\mathrm{C}\langle\lambda_\mathrm{f}|\big)\Big] \neq 1, \tag{5.92}$$

where $I_\mathrm{S} := \sum_\lambda I_\mathrm{I}(\lambda)\otimes|\lambda\rangle_\mathrm{C}\langle\lambda|$ is the identity operator of the thermodynamic system S.

Finally, we show that the equation (5.87) reduces to the case of the cyclic process (5.72) when the control system C has only one eigenstate. In this case, the state of the control system C cannot changes from the initial state, and we thereby obtain $p_{\lambda_\mathrm{i}\to\lambda_\mathrm{i}} = 1$ and $\Delta F_\mathrm{I}(\lambda_\mathrm{i},\lambda_\mathrm{i})$. Therefore, the equation (5.85) reduces to

$$P_{\lambda_\mathrm{i}\to\lambda_\mathrm{f}}(W) = e^{-\beta W}\sum_j \delta\big(W-w_j\big)\mathrm{Tr}\Big[\rho_\mathrm{I}(\lambda_\mathrm{i})\otimes|\lambda_\mathrm{i}\rangle_\mathrm{C}\langle\lambda_\mathrm{i}|\mathcal{K}_j\big(I_\mathrm{I}(\lambda_\mathrm{i})\otimes|\lambda_\mathrm{i}\rangle_\mathrm{C}\langle\lambda_\mathrm{i}|\big)\Big]. \tag{5.93}$$

Because the control system C has only one eigenstate in this case, we obtain $I_\mathrm{S} = I_\mathrm{I}(\lambda_\mathrm{i})\otimes|\lambda_\mathrm{i}\rangle_\mathrm{C}\langle\lambda_\mathrm{i}|$ and $\rho_\mathrm{S} = \rho_\mathrm{I}(\lambda_\mathrm{i})\otimes|\lambda_\mathrm{i}\rangle_\mathrm{C}\langle\lambda_\mathrm{i}|$, and thereby the equation (5.93) is equivalent to the equation (5.70).

5.3 Calculation for a simple model

In this section, we evaluate the coefficient $\gamma_{\lambda_\mathrm{i}\to\lambda_\mathrm{f}}$ of the section 5.2.2 using a simple system. We suppose that the Hamiltonian of the simple thermodynamic system S and the internal system I is given by

$$H_\mathrm{S}(\omega) := \sum_{\lambda=0,1} H_\mathrm{I}(\lambda;\omega)\otimes|\lambda\rangle_\mathrm{C}\langle\lambda|, \tag{5.94}$$

$$H_\mathrm{I}(\lambda;\omega) := \frac{\omega}{2}(\lambda+1)\sigma_z^\mathrm{I}, \tag{5.95}$$

where ω is level spacing and $\sigma_z^\mathrm{I} := |1\rangle_\mathrm{I}\langle 1| - |0\rangle_\mathrm{I}\langle 0|$. The canonical distribution of the internal system I at the inverse temperature β is given by

$$\rho_\mathrm{I}(\tilde{\beta},\lambda) := \sum_{n=0,1}\pi_n(\tilde{\beta},\lambda)|n\rangle_\mathrm{I}\langle n|, \tag{5.96}$$

$$\pi_n(\tilde{\beta},\lambda) := \frac{1}{1+\exp\left((-1)^{(1-n)}(\lambda+1)\tilde{\beta}\right)}, \tag{5.97}$$

where $\tilde{\beta} := \beta\omega$ is the dimensionless inverse temperature.

We suppose that the work extraction process $\mathcal{K}_j$ on the thermodynamic system S is given by the following equation using a unitary operator U_eff:

$$\mathcal{K}_j(\rho_\mathrm{S}) := K_j\rho_\mathrm{S}K_j^\dagger, \tag{5.98}$$

$$K_j := \sum_{\lambda,\lambda'=0,1}\ \sum_{x(\lambda),y(\lambda')=0,1} \delta_{w_j,h_{x(\lambda)}-h_{y(\lambda')}}\Pi_{y(\lambda')}U_\mathrm{eff}\Pi_{x(\lambda)} \tag{5.99}$$

with $h_{x(\lambda)} := (-1)^{1-x(\lambda)}(\lambda+1)\omega/2$ and $\Pi_{x(\lambda)} := |x(\lambda),\lambda\rangle_\mathrm{IC}\langle x(\lambda),\lambda|$. Then, the corresponding time-evolution map $\mathcal{K} := \sum_j \mathcal{K}_j$ is unital and, therefore, is not a feedback process. The unitary operator U_eff is represented as the tracing out the external agent from the time evolution of the total system. We define the effective Hamiltonian by $H_\mathrm{eff} := -T^{-1}\log U_\mathrm{eff}$, where T is the operation time of the work extraction process $\mathcal{K}_j$. For simplicity, we suppose that the effective Hamiltonian H_eff is given by

$$H_\mathrm{eff}(\omega,\xi,\eta) := H_\mathrm{S}(\omega) + V_\mathrm{eff}(\xi\omega) + H_\mathrm{hop}(\eta\omega), \tag{5.100}$$

$$V_\mathrm{eff}(\alpha) := \alpha I_\mathrm{I}\otimes|1\rangle_\mathrm{C}\langle 1|, \tag{5.101}$$

$$H_\mathrm{hop}(\alpha) := \sigma_x^\mathrm{I}\otimes\left(\alpha|1\rangle_\mathrm{C}\langle 0| + \alpha^*|0\rangle_\mathrm{C}\langle 1|\right), \tag{5.102}$$

where the parameters ξ and η are real and complex numbers, respectively, and $\sigma_x^\mathrm{I} := |1\rangle_\mathrm{I}\langle 0| + |0\rangle_\mathrm{I}\langle 1|$. The operators $V_\mathrm{eff}(\alpha)$ and $H_\mathrm{hop}(x)$ represent potential and hopping terms of the effective Hamiltonian H_eff (the figure 5.6). The unitary operator U_eff is rewritten by

$$U_\mathrm{eff}(\xi,\eta,\tilde{T}) := \exp\left(-i\tilde{T}H_\mathrm{eff}(1,\xi,\eta)\right), \tag{5.103}$$

where $\tilde{T} := \omega T/\hbar$ is the dimensionless operation time.

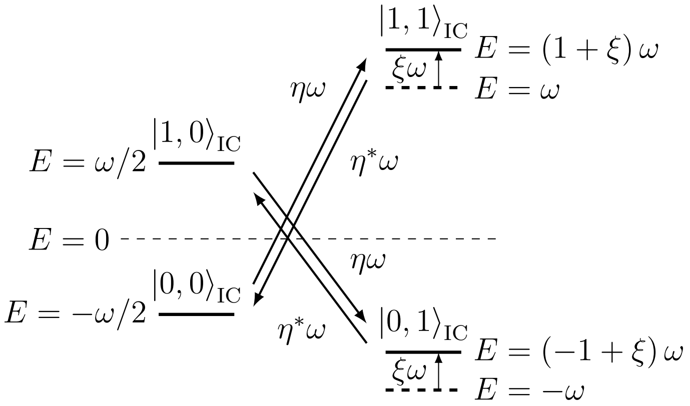

Figure 5.6: Illustration of the effective Hamiltonian of the equation (5.100). The parameter ξ is a real number representing the energy shift by the potential and the parameter η is a complex number representing the hopping amplitude.

Then, the forward and backward transition probabilities (5.84) and (5.89) in the section 5.2.2 are given by

$$p_{\lambda_{\mathrm{i}}\to\lambda_{\mathrm{f}}}(\xi,\eta,\tilde{\beta},\tilde{T}) \coloneqq \sum_{n=0,1} \pi_n(\tilde{\beta},\lambda_{\mathrm{i}})\, p^{(n)}_{\lambda_{\mathrm{i}}\to\lambda_{\mathrm{f}}}(\xi,\eta,\tilde{T}), \tag{5.104a}$$

$$q_{\lambda_{\mathrm{f}}\to\lambda_{\mathrm{i}}}(\xi,\eta,\tilde{\beta},\tilde{T}) \coloneqq \sum_{n=0,1} \pi_n(\tilde{\beta},\lambda_{\mathrm{f}})\, q^{(n)}_{\lambda_{\mathrm{f}}\to\lambda_{\mathrm{i}}}(\xi,\eta,\tilde{T}), \tag{5.104b}$$

with

$$p^{(n)}_{\lambda_{\mathrm{i}}\to\lambda_{\mathrm{f}}}(\xi,\eta,\tilde{T}) \coloneqq \mathrm{Tr}\Big[|\lambda_{\mathrm{f}}\rangle_{\mathrm{C}}\langle\lambda_{\mathrm{f}}| U_{\mathrm{eff}}(\xi,\eta,\tilde{T})\big(|n\rangle_{\mathrm{I}}\langle n| \otimes |\lambda_{\mathrm{i}}\rangle_{\mathrm{C}}\langle\lambda_{\mathrm{i}}|\big) U^{\dagger}_{\mathrm{eff}}(\xi,\eta,\tilde{T})\Big], \tag{5.105a}$$

$$q^{(n)}_{\lambda_{\mathrm{f}}\to\lambda_{\mathrm{i}}}(\xi,\eta,\tilde{T}) \coloneqq \mathrm{Tr}\Big[|\lambda_{\mathrm{i}}\rangle_{\mathrm{C}}\langle\lambda_{\mathrm{i}}| U^{\dagger}_{\mathrm{eff}}(\xi,\eta,\tilde{T})\big(|n\rangle_{\mathrm{I}}\langle n| \otimes |\lambda_{\mathrm{f}}\rangle_{\mathrm{C}}\langle\lambda_{\mathrm{f}}|\big) U_{\mathrm{eff}}(\xi,\eta,\tilde{T})\Big] \tag{5.105b}$$

for $n=0,1$.

Let us calculate the coefficient $\gamma_{\lambda_{\mathrm{i}}\to\lambda_{\mathrm{f}}}$ of the equation (2.10). We now define unitary operators

$$S_1 \coloneqq I_{\mathrm{I}} \otimes \big(|1\rangle_{\mathrm{C}}\langle 1| + e^{i\chi}|0\rangle_{\mathrm{C}}\langle 0|\big), \tag{5.106}$$

$$S_2 \coloneqq \sigma^{\mathrm{I}}_x \otimes I_{\mathrm{C}}, \tag{5.107}$$

where χ is any real number, and a operator K as the complex-conjugate operator. These operators satisfy

$$S_1\,|n,\lambda\rangle_{\mathrm{IC}} = |n,\lambda\rangle_{\mathrm{IC}}\,, \tag{5.108a}$$

$$S_2\,|n,\lambda\rangle_{\mathrm{IC}} = |1-n,\lambda\rangle_{\mathrm{IC}}\,, \tag{5.108b}$$

$$K\,|n,\lambda\rangle_{\mathrm{IC}} = |n,\lambda\rangle_{\mathrm{IC}} \tag{5.108c}$$

for $n = 0, 1$ and $\lambda = 0, 1$, where $|n, \lambda\rangle_{\mathrm{IC}} := |n\rangle_{\mathrm{I}} \otimes |\lambda\rangle_{\mathrm{C}}$. The effective Hamiltonian H_{eff} of the equation (5.100) satisfies

$$S_1 H_{\mathrm{eff}}(\omega, \xi, \eta) S_1^\dagger = H_{\mathrm{eff}}(\omega, \xi, e^{i\chi}\eta), \tag{5.109a}$$

$$S_2 H_{\mathrm{eff}}(\omega, \xi, \eta) S_2^\dagger = -H_{\mathrm{eff}}(\omega, -\xi, -\eta), \tag{5.109b}$$

$$K H_{\mathrm{eff}}(\omega, \xi, \eta) K = H_{\mathrm{eff}}(\omega, \xi, \eta^*), \tag{5.109c}$$

and we thereby obtain

$$S_1 U_{\mathrm{eff}}(\xi, \eta, \tilde{T}) S_1^\dagger = U_{\mathrm{eff}}(\xi, e^{i\chi}\eta, \tilde{T}), \tag{5.110a}$$

$$S_2 U_{\mathrm{eff}}(\xi, \eta, \tilde{T}) S_2^\dagger = U_{\mathrm{eff}}^\dagger(-\xi, -\eta, \tilde{T}), \tag{5.110b}$$

$$K U_{\mathrm{eff}}(\xi, \eta, \tilde{T}) K = U_{\mathrm{eff}}^\dagger(\xi, \eta^*, \tilde{T}). \tag{5.110c}$$

Inserting the equations (5.108) and (5.110) into the equations (5.105), we obtain

$$p^{(n)}_{\lambda_{\mathrm{i}}\to\lambda_{\mathrm{f}}}(\xi, \eta, \tilde{T}) = p^{(n)}_{\lambda_{\mathrm{i}}\to\lambda_{\mathrm{f}}}(\xi, e^{i\chi}\eta, \tilde{T}) \tag{5.111a}$$

$$= q^{(1-n)}_{\lambda_{\mathrm{i}}\to\lambda_{\mathrm{f}}}(-\xi, -\eta, \tilde{T}) \tag{5.111b}$$

$$= q^{(n)}_{\lambda_{\mathrm{i}}\to\lambda_{\mathrm{f}}}(\xi, \eta^*, \tilde{T}). \tag{5.111c}$$

As can be seen from the above equations, the equations (5.105) do not depend on the phase of the parameter η, and we obtain

$$p^{(n)}_{\lambda_{\mathrm{i}}\to\lambda_{\mathrm{f}}}(\xi, |\eta|, \tilde{T}) = p^{(n)}_{\lambda_{\mathrm{i}}\to\lambda_{\mathrm{f}}}(\xi, \eta, \tilde{T}) \tag{5.112a}$$

$$= p^{(1-n)}_{\lambda_{\mathrm{i}}\to\lambda_{\mathrm{f}}}(-\xi, \eta, \tilde{T}) \tag{5.112b}$$

$$= q^{(n)}_{\lambda_{\mathrm{i}}\to\lambda_{\mathrm{f}}}(\xi, \eta, \tilde{T}). \tag{5.112c}$$

Therefore, we obtain

$$\begin{aligned} p_{\lambda_{\mathrm{i}}\to\lambda_{\mathrm{f}}}(\xi, \eta, \tilde{\beta}, \tilde{T}) &= q_{\lambda_{\mathrm{i}}\to\lambda_{\mathrm{f}}}(\xi, \eta, \tilde{\beta}, \tilde{T}) \\ &= \sum_{n=0,1} \pi_n(\tilde{\beta}, \lambda_{\mathrm{i}}) p^{(0)}_{\lambda_{\mathrm{i}}\to\lambda_{\mathrm{f}}}((-1)^n\xi, |\eta|, \tilde{T}), \end{aligned} \tag{5.113}$$

and hence

$$\gamma_{\lambda_{\mathrm{i}}\to\lambda_{\mathrm{f}}}(\xi, \eta, \tilde{\beta}, \tilde{T}) := \frac{q_{\lambda_{\mathrm{f}}\to\lambda_{\mathrm{i}}}(\xi, \eta, \tilde{\beta}, \tilde{T})}{p_{\lambda_{\mathrm{i}}\to\lambda_{\mathrm{f}}}(\xi, \eta, \tilde{\beta}, \tilde{T})} = \frac{p_{\lambda_{\mathrm{f}}\to\lambda_{\mathrm{i}}}(\xi, \eta, \tilde{\beta}, \tilde{T})}{p_{\lambda_{\mathrm{i}}\to\lambda_{\mathrm{f}}}(\xi, \eta, \tilde{\beta}, \tilde{T})}. \tag{5.114}$$

As can be seen from the above result, the coefficient $\gamma_{\lambda_{\mathrm{i}}\to\lambda_{\mathrm{f}}}$ satisfies $\gamma_{1\to 0} = 1/\gamma_{0\to 1}$, and is always equal to unity if $\lambda_{\mathrm{i}} = \lambda_{\mathrm{f}}$, namely, $\gamma_{0\to 0} = \gamma_{1\to 1} = 1$.

Let us find $\gamma_{1\to 0}$. Calculating $p_{1\to 0}(\xi, \eta, \tilde{\beta}, \tilde{T})$ and $p_{0\to 1}(\xi, \eta, \tilde{\beta}, \tilde{T})$, we obtain

$$p_{1\to 0}(\xi, \eta, \tilde{\beta}, \tilde{T}) = p_{0\to 1}(-\xi, \eta, \tilde{\beta}, \tilde{T}) = |\eta|^2 \tilde{T}^2 \mathrm{sinc}^2(f(\xi, |\eta|)\tilde{T}) \tag{5.115}$$

with

$$\operatorname{sinc}(x) := \frac{\sin(x)}{x}, \tag{5.116}$$

$$f(\xi, |\eta|) := \sqrt{|\eta|^2 + \left(\frac{3-2\xi}{4}\right)^2}. \tag{5.117}$$

Inserting the equation (5.115) into the equation (5.113), we obtain

$$\begin{aligned}
p_{1\to 0}(\xi, \eta, \tilde{\beta}, \tilde{T}) &= |\eta|^2 \tilde{T}^2 \sum_{n=0,1} \pi_n(\tilde{\beta}, 0)\operatorname{sinc}^2\big(f((-1)^n \xi, |\eta|)\tilde{T}\big) \\
&= |\eta|^2 \tilde{T}^2 \left[\frac{\operatorname{sinc}^2\big(f(\xi, |\eta|)\tilde{T}\big)}{1+e^{-2\tilde{\beta}}} + \frac{\operatorname{sinc}^2\big(f(-\xi, |\eta|)\tilde{T}\big)}{1+e^{2\tilde{\beta}}}\right],
\end{aligned} \tag{5.118}$$

$$\begin{aligned}
p_{0\to 1}(\xi, \eta, \tilde{\beta}, \tilde{T}) &= |\eta|^2 \tilde{T}^2 \sum_{n=0,1} \pi_n(\tilde{\beta}, 1)\operatorname{sinc}^2\big(f((-1)^n \xi, |\eta|)\tilde{T}\big) \\
&= |\eta|^2 \tilde{T}^2 \left[\frac{\operatorname{sinc}^2\big(f(\xi, |\eta|)\tilde{T}\big)}{1+e^{-\tilde{\beta}}} + \frac{\operatorname{sinc}^2\big(f(-\xi, |\eta|)\tilde{T}\big)}{1+e^{\tilde{\beta}}}\right].
\end{aligned} \tag{5.119}$$

We thereby plotted $\gamma_{1\to 0}$ in the figures 5.7. The coefficient $\gamma_{1\to 0}$ wildly fluctuates around unity, even exceeding unity often. This fluctuation of $\gamma_{\lambda_{\mathrm{i}}\to\lambda_{\mathrm{f}}}$ should be detectable in experiments and provide evidence for the conventional derivation.

The conditions for $\gamma_{1\to 0} = 1$ are $\tilde{\beta} = 0$ or the parameters ξ and η satisfying

$$\operatorname{sinc}^2\big(f(\xi, |\eta|)\tilde{T}\big) = \operatorname{sinc}^2\big(f(-\xi, |\eta|)\tilde{T}\big) \tag{5.120}$$

which does not depend on the dimensionless inverse temperature $\tilde{\beta}$ (the figures 5.7(b) and 5.7(c)).

5.4 Summary of this chapter

In this chapter, we have demonstrated the problem of the conventional approach of quantum thermodynamic using the two-level system and derived the quantum version of the Jarzynski equality using the new formulation of the work extraction.

For the demonstration in the section 5.1, we have shown that the variance of the energy obtained by the external agent diverges when the time evolution of the thermodynamic system is approximated to a unitary one. Because of this, the conventional approach, which assumes the unitary dynamics of the thermodynamic system, is unsuitable for quantum thermodynamics and we have to adopt the new formulation of the work extraction.

In the section 5.2, we have adopted the measurement-based work extraction introduced in the chapter 4 as the new formulation of the work extraction and shown the difference between the conventional approach and the measurement-based work extraction using the Jarzynski equality. As a result, the difference between the two approach appears in

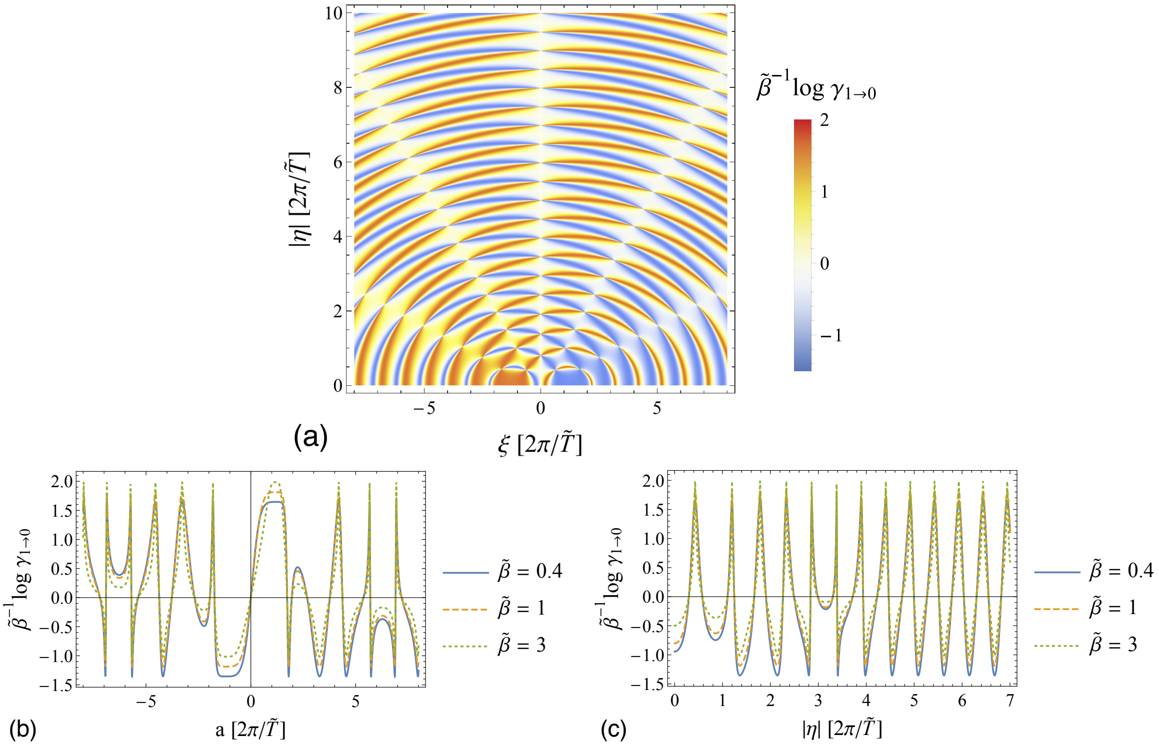

Figure 5.7: (a) Dependence of $\tilde{\beta}^{-1}\log\gamma_{1\to 0}$ on the parameters ξ and $|\eta|$ for the dimensionless operation time $\tilde{T} = 5$ and the dimensionless inverse temperature $\tilde{\beta} = 0.4$. Its cross sections for (b) $|\eta| = 4\pi/5$ and (c) $\xi = 6\pi/5$. The unity of $\gamma_{1\to 0}$ (namely, the zero of $\log\gamma_{1\to 0}$) does not depend on the dimensionless inverse temperature $\tilde{\beta}$.

the coefficient γ of the equation (5.72) in the cyclic process and the coefficient $\gamma_{\lambda_\mathrm{i}\to\lambda_\mathrm{f}}$ of the equation (5.87) in the non-cyclic process. Both coefficients are not generally equal to unity in contrast to the case of the conventional approach, in which the coefficients were always equal to unity. This difference is caused by describing the work extraction in terms of the quantum measurement process. In the case of the cyclic process, the coefficient γ is equal to unity if and only if the time evolution is a "natural" thermodynamic process, in other works, the time-evolution map is a unital. On the other hand, in the case of the non-cyclic process, the coefficient $\gamma_{\lambda_\mathrm{i}\to\lambda_\mathrm{f}}$ does not generally become unity when the time evolution is a "natural" thermodynamic process and widely fluctuates around unity in a simple model of the section 5.3. This fluctuation can be expected to be detected experimentally and can provide evidence for the present approach.

Chapter 6

Quantum Fluctuation theorem under continuously monitored control parameter

In the previous chapter, we derived a quantum version of the Jarzynski equality using the new formulation of work extraction in order to compare the conventional approach and new formulation. As a result, we obtain the difference between the two approaches.

Note that the following difference exists between the work extraction processes in the two approaches: the conventional approach clearly describes the motion of the controller, such as a piston, because its motion is represented by a time-dependent parameter; on the other hand, the new formulation in the section 5.2.2 does not clearly describe one because we do not observe a control system except at the beginning and the end of the work extraction them. Using the piston of a cylinder as an example, in the conventional approach, we can distinguish between pushing the piston after pulling it and pulling it after pushing; on the other hand, in the new formulation, we cannot distinguish.

In order to compare the two approaches under the more similar situations, we here introduce the continuous measurement of the control system and derive another quantum version of the Jarzynski equality for it.

In this chapter, we continuously observe a physical quantity of the control system to describe the operation received the internal system and derive a quantum version of the Jarzynski equality and the second law under this observation. To use for the derivation, we first show time reversal introduced by Åberg [121]. We next derive a fluctuation relation under the continuously monitoring process using Åberg's time reversal. After that, we derive the Jarzynski equality under the continuously monitoring the control parameter. Finally, we show the relation between the parameter change given the continuously monitoring process and the second law of thermodynamics.

The contents of this chapter except the section 6.1.1 are the present results of the author under the collaboration with Dr. H. Tajima.

6.1 Time reversal of completely positive map

6.1.1 Åberg's time reversal

In the standard quantum mechanics, time-reversal transformation for a state vector is given by an antiunitary operator. In contrast, Åberg [121] defined a time-reversal map as a linear map $\mathcal{T}$ satisfying the following conditions [121]:

$$\mathcal{T}(AB) = \mathcal{T}(B)\mathcal{T}(A), \tag{6.1a}$$

$$\mathcal{T}(A^\dagger) = (\mathcal{T}(A))^\dagger, \tag{6.1b}$$

$$\mathrm{Tr}[\mathcal{T}(\rho)] = \mathrm{Tr}[\rho], \tag{6.1c}$$

$$\mathcal{T}^2 = \mathcal{I}, \tag{6.1d}$$

where A and B are bounded operators, ρ is a trace-class operator, Tr denotes the trace and $\mathcal{I}$ is the identity map. Then we can derive the following properties of the time-reversal map $\mathcal{T}$ [121]:

1. For the identity operator I, it satisfies $\mathcal{T}(I) = I$.
2. When an operator Q is positive, $\mathcal{T}(Q)$ is also positive.
3. When an operator U is a unitary operator, $\mathcal{T}(U)$ is also a unitary one.
4. When an operator P is a projection, $\mathcal{T}(P)$ is also a projection. Furthermore, when the projection Q is orthogonal to P, $\mathcal{T}(Q)$ is orthogonal to $\mathcal{T}(P)$.
5. Let $\mathcal{T}_A$ and $\mathcal{T}_B$ denote the time-reversal map on the systems A and B, respectively. Then, the following is satisfied: $\mathrm{Tr}_\mathrm{B}[(\mathcal{T}_A \otimes \mathcal{T}_B)(O_\mathrm{AB})] = \mathcal{T}_A(\mathrm{Tr}_\mathrm{B} O_\mathrm{AB})$, where Tr_B is the partial trace over the system B and O_AB is any operator on the composite system AB.

As can be seen from the condition (6.1a), the time-reversal map $\mathcal{T}$ has a property of the transpose. For a finite-dimensional system, let T denote the transpose defined by

$$A^T := \sum_{n,n'} \langle \psi_{n'} \,|\, A \,|\, \psi_n \rangle \, |\psi_n\rangle\langle\psi_{n'}|, \tag{6.2}$$

where A is an arbitrary operator and $\{\, |\psi_n\rangle \,\}_n$ is an orthonormal basis set. Note that the transpose depends on the choice of orthonormal basis. When T' denotes the transpose defined with respect to another orthogonal basis set $\{\, |\phi_n\rangle \,\}_n$ and a unitary operator W is a transformation from $\{\, |\psi_n\rangle \,\}_n$ to $\{\, |\phi_n\rangle \,\}_n$, the relation between two transposes is given by [121]

$$A^{T'} = WW^T A^T (WW^T)^\dagger. \tag{6.3}$$

The time-reversal map $\mathcal{T}$ can be represented by [121]

$$\mathcal{T}(A) = UA^T U^\dagger, \tag{6.4}$$

where T is the transpose defined with respect to $\{\,|\psi_n\rangle\,\}_n$ and U is a unitary operator uniquely determined by $\mathcal{T}$ and $\{\,|\psi_n\rangle\,\}_n$.

Let us describe the reason of calling the linear map $\mathcal{T}$ as "time reversal". We assume that a system is a quantum closed one with the Hamiltonian H. Let ρ_i denote the initial state of its time evolution. Then, the state ρ_f after time t is given by

$$\rho_\mathrm{f} := U\rho_\mathrm{i}U^\dagger \tag{6.5}$$

with $U := e^{-iHt/\hbar}$. Using the conditions (6.1a) and (6.1b), we obtain

$$\mathcal{T}(\rho_\mathrm{f}) = \mathcal{T}\big(U\rho_\mathrm{i}U^\dagger\big) = \mathcal{T}(U)^\dagger\mathcal{T}(\rho_\mathrm{i})\mathcal{T}(U). \tag{6.6}$$

From the condition (6.1c) and the property 2, $\mathcal{T}(\rho_\mathrm{i})$ and $\mathcal{T}(\rho_\mathrm{f})$ are states, too. Moreover, from the property 3, the time-reversed unitary operator U is a unitary operator. Therefore, we obtain

$$\mathcal{T}(\rho_\mathrm{i}) = \mathcal{T}(U)\mathcal{T}(\rho_\mathrm{f})\mathcal{T}(U)^\dagger. \tag{6.7}$$

This equation describes the unitary evolution from the time-reversed final state $\mathcal{T}(\rho_\mathrm{f})$ to the time-reversed initial one $\mathcal{T}(\rho_\mathrm{i})$ under the unitary operator $\mathcal{T}(U)$. In particular, if the map $\mathcal{T}$ satisfies $\mathcal{T}(H) = H$, which means that the Hamiltonian is invariant under the time reversal, the time-reversed unitary operator $\mathcal{T}(U)$ satisfies $\mathcal{T}(U) = U$. Then, the equation (6.7) becomes

$$\mathcal{T}(\rho_\mathrm{i}) = U\mathcal{T}(\rho_\mathrm{f})U^\dagger. \tag{6.8}$$

This equation describes the forward unitary evolution from the time-reversed final state $\mathcal{T}(\rho_\mathrm{f})$ to the time-reversed initial one $\mathcal{T}(\rho_\mathrm{i})$. Hence, the linear map $\mathcal{T}$ satisfying the conditions (6.1) represents a time-reversal operation.

We note that the conditions (6.1) are not the most general definition of the time reversal [121]. For the standard quantum mechanics, the time reversal is represented by an antiunitary operator Θ [13]. The corresponding map is given by $\mathcal{T}_\Theta(\rho) := \Theta\rho\Theta^\dagger$. However, the map $\mathcal{T}_\Theta$ is an antilinear map, not a linear map. Therefore, the map $\mathcal{T}_\Theta$ does not satisfies the conditions (6.1).

We now rewrite the equation (6.5) as

$$\rho_\mathrm{f} = \mathcal{U}(\rho_\mathrm{i}), \tag{6.9}$$

where the map $\mathcal{U}$ is a unitary time-evolution map with respect to the unitary operator U and is given by $\mathcal{U}(\rho) := U\rho U^\dagger$ for any state ρ. Then, we can rewrite the time-reversed unitary evolution of the equation (6.8) as

$$\mathcal{T}(\rho_\mathrm{i}) = \mathcal{U}^\ominus(\mathcal{T}(\rho_\mathrm{f})), \tag{6.10}$$

where $\ominus$ is defined by

$$\phi^\ominus := \mathcal{T}\phi^\dagger\mathcal{T} \tag{6.11}$$

for any completely positive (CP) map ϕ [121]. Therefore, the translation from a time evolution to a time-reversed one is represented by the $\ominus$ translation of the equation (6.11).

6.1.2 Time reversal of continuous measurement

Can we obtain a time-reversed continuous measurement from the $\ominus$ translation? To consider the continuous measurement, we first show the $\ominus$ translation of the general measurement process. Let $\mathcal{M}_a$ denote a measurement process with respect to a specific outcome a and is given by an indirect measurement model in the form

$$\mathcal{M}_a(\rho) := \mathrm{Tr}_{\mathrm{D}}\big[(I_{\mathrm{S}} \otimes P_a^{\mathrm{D}})U(\rho \otimes \sigma_{\mathrm{D}})U^{\dagger}\big], \tag{6.12}$$

where Tr_{D}, ρ, I_{S}, P_a^{D}, σ_{D} and U are the partial trace over a measurement device D, ρ is an initial state of a system of interest S, the identity operator of S, an projection of specific eigenvalue a of a meter observable A_{D} on D, an initial state of D, and an unitary operator on the total system, respectively The adjoint of a completely positive (CP) map given in the appendix A gives

$$\mathcal{M}_a^{\dagger}(\rho) := \mathrm{Tr}_{\mathrm{D}}\big[(I_{\mathrm{S}} \otimes \sigma_{\mathrm{D}})U^{\dagger}(\rho \otimes P_a^{\mathrm{D}})U\big]. \tag{6.13}$$

and thereby obtain

$$\begin{aligned}
\mathcal{M}_a^{\ominus}(\rho) &= \mathcal{T} \circ \mathcal{M}_a^{\dagger} \circ \mathcal{T}(\rho) &\quad (6.14)\\
&= \mathrm{Tr}_{\mathrm{D}}\big[\mathcal{T}_{\mathrm{SD}}\big((I_{\mathrm{S}} \otimes \sigma_{\mathrm{D}})U^{\dagger}(\mathcal{T}(\rho) \otimes P_a^{\mathrm{D}})U\big)\big] &\quad (6.15)\\
&= \mathrm{Tr}_{\mathrm{D}}\big[(I_{\mathrm{S}} \otimes \mathcal{T}_{\mathrm{D}}(\sigma_{\mathrm{D}}))\mathcal{T}_{\mathrm{SD}}(U)(\rho \otimes \mathcal{T}_{\mathrm{D}}(P_a^{\mathrm{D}}))\mathcal{T}_{\mathrm{SD}}(U)^{\dagger}\big], &\quad (6.16)
\end{aligned}$$

where $\mathcal{T}$ and $\mathcal{T}_{\mathrm{D}}$ are the time-reversal map on the system of interest S and the measurement device D, respectively, and $\mathcal{T}_{\mathrm{SD}} := \mathcal{T} \otimes \mathcal{T}_{\mathrm{D}}$. From the condition (6.1c) and the properties (2), (3) and (4) of the time-reversal map in the section 6.1.1, the operators $\mathcal{T}_{\mathrm{D}}\sigma$, $\mathcal{T}_{\mathrm{SD}}(U)$ and $\mathcal{T}_{\mathrm{D}}P_a^{\mathrm{D}}$ are also a state of D, a unitary operator of the total system and a projection on D, respectively. Defining another measurement process given by

$$\tilde{\mathcal{M}}_a(\rho) := \mathrm{Tr}_{\mathrm{D}}\big[(I_{\mathrm{S}} \otimes \mathcal{T}_{\mathrm{D}}(P_a^{\mathrm{D}}))\mathcal{T}_{\mathrm{SD}}(U)^{\dagger}(\rho \otimes \mathcal{T}_{\mathrm{D}}(\sigma_{\mathrm{D}}))\mathcal{T}_{\mathrm{SD}}(U)\big] = \mathcal{T} \circ \mathcal{M}_a \circ \mathcal{T}(\rho), \tag{6.17}$$

we obtain

$$\mathcal{M}_a^{\ominus} = \tilde{\mathcal{M}}_a^{\dagger}. \tag{6.18}$$

Therefore, the $\ominus$ translation of the measurement process becomes the adjoint of another measurement process. In general, the adjoint of the measurement process is not a measurement process, because, the summation of the adjoint of the measurement processes does not satisfy the trace preserving. However, when the summation is a unital map, the adjoint of the measurement process becomes a measurement process. Hence, the $\ominus$ translation of the measurement process $\mathcal{M}_a^{\ominus}$ is a measurement process if and only if the summation $\sum_a \mathcal{M}_a$ is a unital map.

Let us consider the $\ominus$ transformation of the continuous measurement. From the section 2.2.3, the continuous measurement with respect to a measurement record $[a] := \{\, a(t) \mid t \in (0, T) \,\}$, where $a(t)$ is a path of the measurement outcome, is given by

$$\begin{aligned}
\mathcal{M}_{[a]} := \lim_{N\to\infty} \mathcal{U}_{t_N,t_{N-1}}\, \mathcal{M}_{a_{N-1},t_{N-1}}\, \mathcal{U}_{t_{N-1},t_{N-2}}\, \mathcal{M}_{a_{N-2},t_{N-2}}&\\
\times \cdots \times \mathcal{U}_{t_2,t_1}\, \mathcal{M}_{a_1,t_1}\, \mathcal{U}_{t_1,t_0},&
\end{aligned} \tag{6.19}$$

where $\mathcal{U}_{s,t}$ is a unitary evolution given by a unitary operator $U(s,t)$ from time t to s, $\mathcal{M}_{a,t}$ is an instantaneous measurement process at time t with respect to a specific outcome a, $t_n := nT/N$ and $a_n := a(t_n)$. To operator the $\ominus$ translation to the continuous measurement of the equation (6.19), we obtain

$$\mathcal{M}^{\ominus}_{[a]} := \lim_{N\to\infty} \mathcal{U}^{\ominus}_{t_1 t_0} \mathcal{M}^{\ominus}_{a_1,t_1} \mathcal{U}^{\ominus}_{t_2,t_1} \mathcal{M}^{\ominus}_{a_2,t_2} \times \cdots \times \mathcal{U}^{\ominus}_{t_{N-1},t_{N-2}} \mathcal{M}^{\ominus}_{a_{N-1},t_{N-1}} \mathcal{U}^{\ominus}_{t_N,t_{N-1}}, \tag{6.20}$$

where we use the property $(\phi\chi)^{\ominus} = \chi^{\ominus}\phi^{\ominus}$ of the $\ominus$ translation.

For simplify, we assume that the time-reversal map $\mathcal{T}$ satisfies $\mathcal{T}(U(s,t)) = U(s,t)$ for any time t and s. Then, the unitary evolution $\mathcal{U}_{s,t}$ is the invariant under the $\ominus$ translation:

$$\mathcal{U}^{\ominus}_{s,t} = \mathcal{U}_{s,t}. \tag{6.21}$$

In the other hand, from the equation (6.18), $\mathcal{M}^{\ominus}_{a,t}$ is the adjoint of another measurement process $\tilde{\mathcal{M}}^{\dagger}_{a,t}$. Hence, the $\ominus$ translation of the continuous measurement (6.19) is given by

$$\mathcal{M}^{\ominus}_{[a]} := \lim_{N\to\infty} \mathcal{U}_{t_1 t_0} \tilde{\mathcal{M}}^{\dagger}_{a_1,t_1} \mathcal{U}_{t_2,t_1} \tilde{\mathcal{M}}^{\dagger}_{a_2,t_2} \times \cdots \times \mathcal{U}_{t_{N-1},t_{N-2}} \tilde{\mathcal{M}}^{\dagger}_{a_{N-1},t_{N-1}} \mathcal{U}_{t_N,t_{N-1}}. \tag{6.22}$$

As we can see the equation (6.22), the orders of unitary evolutions $\mathcal{U}_{(t_n,t_{n-1})}$ and the (instantaneous) outcomes a_n is a time-reversed one, however, $\tilde{\mathcal{M}}^{\dagger}_{a}$ is not a (instantaneous) measurement process. Hence, the $\ominus$ translation of the continuous measurement is a backward-like map, not a backward continuous measurement. Here, the "backward" means that the measurement record is the reverse order given by $[\tilde{a}] := \{\, \tilde{a}(t) \mid t \in (0,T) \,\}$ with $\tilde{a}(t) := a(T-t)$.

6.2 Fluctuation relation under continuously monitoring process

We consider the fluctuation relation of a work extraction process with continuously monitored control parameter. Let us consider a quantum closed system including an internal system I, a control system C and an external agent E. The internal system is controlled by a physical quantity Λ of the control system C, which is regarded as a control parameter of the internal system I. The external agent E interacts with the composite system IC of the internal system I and the control system C, and receives the energy as the work. We assume that the interaction between the composite system IC and the external agent E is activated from time 0 to T and is deactivated the other times. To monitor the change of the control parameter, we measure the physical quantity Λ during the interaction (the figure 6.1).

Let H_{IC} and H_{E} denote the Hamiltonian of the composite system IC and the external agent E, respectively. We assume that the Hamiltonian H_{IC} of the composite system IC is given by

$$H_{\mathrm{IC}} := \sum_{\lambda} H_{\mathrm{I}}(\lambda) \otimes |\lambda\rangle_{\mathrm{C}}\langle\lambda|, \tag{6.23}$$

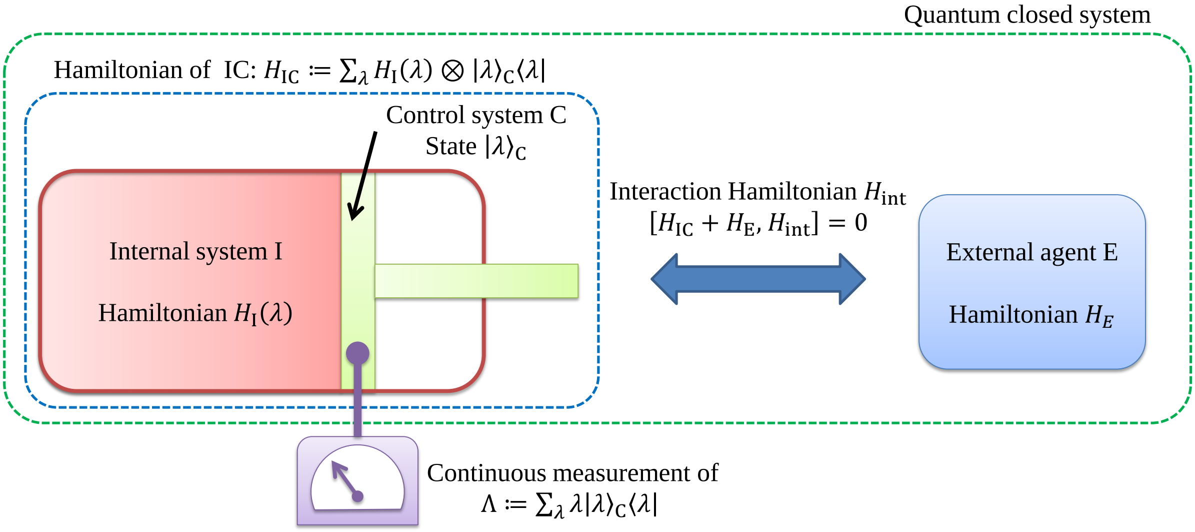

Figure 6.1: Illustration of the quantum closed system in the section 6.2. The quantum closed system is composed by three subsystems; an internal system I, a control system C and an external agent E. The continuous measurement of the physical quantity Λ of the control system C is represented by the repetition of the instantaneous measurement $\{\,\mathcal{M}_\lambda\,\}_\lambda$ of the physical quantity λ (see the equation (6.31)).

where $H_{\mathrm{I}}(\lambda)$ is the Hamiltonian of the internal system I depending on a specific eigenvalue λ of the physical quantity Λ and $|\lambda\rangle$ is the corresponding eigenstate. According to this Hamiltonian, the Hamiltonian of the internal system I is controlled by the state of the control system (see the section 4.2). We assume that the initial state of the composite system IC is the canonical distribution of the internal system I with a pure state $|\lambda_{\mathrm{i}}\rangle$ of the control system C:

$$\rho_{\mathrm{IC}}(\lambda_{\mathrm{i}}) := \frac{e^{-\beta H_{\mathrm{I}}(\lambda_{\mathrm{i}})}}{Z_{\mathrm{I}}(\lambda_{\mathrm{i}})} \otimes |\lambda_{\mathrm{i}}\rangle_{\mathrm{C}}\langle\lambda_{\mathrm{i}}|, \tag{6.24}$$

where β is an inverse temperature and $Z_{\mathrm{I}}(\lambda_{\mathrm{i}}) := \mathrm{Tr}\big[e^{-\beta H_{\mathrm{I}}(\lambda_{\mathrm{i}})}\big]$ is the partition function. The corresponding Helmholtz free energy is given by $F_{\mathrm{I}}(\lambda_{\mathrm{i}}) := -\beta^{-1}\log Z_{\mathrm{I}}(\lambda_{\mathrm{i}})$.

Let H_{int} denote the interaction Hamiltonian between the composite system IC and the external agent E. The Hamiltonian of the total system between time 0 and T is given by

$$H_{\mathrm{tot}} := H_{\mathrm{IC}} + H_{\mathrm{E}} + H_{\mathrm{int}}, \tag{6.25}$$

and the time evolution of the total system from time t to t' ($t, t' \in [0, T]$) without measurement is given by the unitary operator

$$U(t'-t) := \exp\left[-\frac{i}{\hbar} H_{\mathrm{tot}}(t'-t)\right]. \tag{6.26}$$

We here assume that the interaction Hamiltonian H_{int} satisfies the energy conservation in the from

$$[H_{\mathrm{IC}} + H_{\mathrm{E}}, H_{\mathrm{int}}] = 0. \tag{6.27}$$

Then, the unitary operator U satisfies the energy conservation

$$[H_{\mathrm{IC}} + H_{\mathrm{E}}, U(t)] = 0 \tag{6.28}$$

for $t \in [0, T]$.

Let us measure the physical quantity Λ of the control system during the interaction to monitor the change of the control parameter, using the continuous measurement in the section 2.2.3. Let $\{ \mathcal{M}_\lambda \}_\lambda$ denote the set of the instrument measurement of the physical quantity Λ on the total system. We assume the energy conservation

$$\left[H_{\mathrm{IC}} + H_{\mathrm{E}}, M_{n,\lambda}\right] = 0 \tag{6.29}$$

for all measurement outcomes λ and any integral n, where $\{ M_{n,\lambda} \}_n$ is the set of the Kraus operator of $\mathcal{M}_\lambda$ given by $\mathcal{M}_\lambda(\rho) = \sum_n M_{n,\lambda}\rho M_{n,\lambda}^\dagger$. This means that the measurement processes $\{ \mathcal{M}_\lambda \}_\lambda$ do not cause a net energy transfer and the energy extracted by the external agent E only comes from the composite system IC. The energy conservation (6.29) gives

$$\mathcal{M}_\lambda \mathcal{P}_{H_{\mathrm{IC}}+H_{\mathrm{E}},h} = \mathcal{P}_{H_{\mathrm{IC}}+H_{\mathrm{E}},h} \mathcal{M}_\lambda \tag{6.30}$$

for all outcomes λ and all eigenvalues h of $H_{\mathrm{IC}} + H_{\mathrm{E}}$, where a map $\mathcal{P}_{A,a}$ of a Hermitian operator A and the eigenvalue a of A is defined by $\mathcal{P}_{A,a}(\bullet) := P_a \bullet P_a$ with the projection P_a of the eigenvalue a.

We define the continuous measurement of the physical quantity Λ with respect to a specific measurement record $[\lambda] := \{ \lambda(t) \mid t \in (0, T) \}$, where $\lambda(t)$ is a path of the measurement outcome, in the total system by

$$\mathcal{M}_{[\lambda]} := \lim_{N\to\infty} \mathcal{U}_\tau \mathcal{M}_{\lambda_{n-1}} \mathcal{U}_\tau \mathcal{M}_{\lambda_{n-2}} \times \cdots \times \mathcal{U}_\tau \mathcal{M}_{\lambda_1} \mathcal{U}_\tau \tag{6.31}$$

with $\tau := T/N$, $\lambda_n := \lambda(nT/N)$ and $\mathcal{U}_t(\rho) := U(t)\rho U^\dagger(t)$. Because of the energy conservations of the equations (6.28) and (6.30), the continuous measurement $\mathcal{M}_{[\lambda]}$ satisfies

$$\mathcal{M}_{[\lambda]} \mathcal{P}_{H_{\mathrm{IC}}+H_{\mathrm{E}},h} = \mathcal{P}_{H_{\mathrm{IC}}+H_{\mathrm{E}},h} \mathcal{M}_{[\lambda]} \tag{6.32}$$

for any measurement record $[\lambda]$ and all eigenvalue h of $H_{\mathrm{IC}} + H_{\mathrm{E}}$, and thereby we obtain

$$\mathcal{M}_{[\lambda]} \mathcal{J}_{\alpha(H_{\mathrm{IC}}+H_{\mathrm{E}})} = \mathcal{J}_{\alpha(H_{\mathrm{IC}}+H_{\mathrm{E}})} \mathcal{M}_{[\lambda]} \tag{6.33}$$

for any real number α and any measurement recored $[\lambda]$, where the map $\mathcal{J}_A$ is defined by $\mathcal{J}_A(\bullet) := e^{-A/2} \bullet e^{-A/2}$.

Let $\mathcal{T}_{\mathrm{IC}}$ and $\mathcal{T}_{\mathrm{E}}$ denote time-reversal maps on the composite system IC and the external agent E, respectively. We assume that the time-reversal maps do not change the Hamiltonians:

$$\mathcal{T}_{\mathrm{IC}}(H_{\mathrm{IC}}) = H_{\mathrm{IC}}, \tag{6.34}$$

$$\mathcal{T}_{\mathrm{E}}(H_{\mathrm{E}}) = H_{\mathrm{E}}, \tag{6.35}$$

$$(\mathcal{T}_{\mathrm{IC}} \otimes \mathcal{T}_{\mathrm{E}})(H_{\mathrm{int}}) = H_{\mathrm{int}}. \tag{6.36}$$

Then, the unitary operator $U(t)$ of the equation (6.26) satisfies $\mathcal{T}(U(t)) = U(t)$. As in the section 6.1.2, we define the backward-like map of the continuous measurement (6.31) by

$$\tilde{\mathcal{M}}_{[\tilde{\lambda}]} := \mathcal{M}^{\ominus}_{[\lambda]} = \lim_{N\to\infty} \mathcal{U}_\tau \tilde{\mathcal{M}}_{\tilde{\lambda}_{n-1}} \mathcal{U}_\tau \tilde{\mathcal{M}}_{\tilde{\lambda}_{n-2}} \times \cdots \times \mathcal{U}_\tau \tilde{\mathcal{M}}_{\tilde{\lambda}_1} \mathcal{U}_\tau, \tag{6.37}$$

where $\tilde{\mathcal{M}}_a := \mathcal{T}\mathcal{M}_a\mathcal{T}$, $\left[\tilde{\lambda}\right] := \left\{\, \tilde{\lambda}(t) \mid t \in (0,T) \,\right\}$ with $\tilde{\lambda}(t) := \lambda(T-t)$ and $\tilde{\lambda}_n := \tilde{\lambda}(n\tau)$.

From the above setup, let us derive the fluctuation relation under the continuously monitoring process. The initial state of the composite system IC of the equation (6.24) and the continuous measurement on the total system of the equation (6.31) yield the continuous measurement in the external agent E in the form

$$\mathcal{F}_{\lambda_\mathrm{f},[\lambda],\lambda_\mathrm{i}}(\sigma) := \mathrm{Tr}_\mathrm{IC}\Big[|\lambda_\mathrm{f}\rangle_\mathrm{C}\langle\lambda_\mathrm{f}|\mathcal{M}_{[\lambda]}(\rho_\mathrm{IC}(\lambda_\mathrm{i}) \otimes \sigma)\Big] \tag{6.38}$$

for an arbitrary initial state σ of the external agent E. Using the equation (6.37), we define the backward-like map on the external agent E by

$$\mathcal{R}_{\tilde{\lambda}_\mathrm{f},[\tilde{\lambda}],\tilde{\lambda}_\mathrm{i}}(\sigma) := \mathrm{Tr}_\mathrm{IC}\Big[|\tilde{\lambda}_\mathrm{i}\rangle_\mathrm{C}\langle\tilde{\lambda}_\mathrm{i}|\tilde{\mathcal{M}}_{[\tilde{\lambda}]}(\rho_\mathrm{IC}(\tilde{\lambda}_\mathrm{f}) \otimes \sigma)\Big], \tag{6.39}$$

where $I_\mathrm{I} \otimes |\tilde{\lambda}_\alpha\rangle_\mathrm{C}\langle\tilde{\lambda}_\alpha| := \mathcal{T}_\mathrm{IC}\big(I_\mathrm{I} \otimes |\lambda_\alpha\rangle_\mathrm{C}\langle\lambda_\alpha|\big)$ for $\alpha = \mathrm{i}, \mathrm{f}$.

From the equation (6.33), we obtain

$$\begin{aligned}\mathcal{M}_{[\lambda]}(\rho_\mathrm{IC}(\lambda_\mathrm{i}) \otimes \sigma) &= \frac{1}{Z_\mathrm{I}(\lambda_\mathrm{i})}\mathcal{M}_{[\lambda]} \circ \mathcal{J}_{\beta(H_\mathrm{IC}+H_\mathrm{E})}\big(|\lambda_\mathrm{i}\rangle_\mathrm{C}\langle\lambda_\mathrm{i}| \otimes \mathcal{J}^{-1}_{\beta H_\mathrm{E}}(\sigma)\big) &(6.40)\\ &= \frac{1}{Z_\mathrm{I}(\lambda_\mathrm{i})}\mathcal{J}_{\beta(H_\mathrm{IC}+H_\mathrm{E})} \circ \mathcal{M}_{[\lambda]}\big(|\lambda_\mathrm{i}\rangle_\mathrm{C}\langle\lambda_\mathrm{i}| \otimes \mathcal{J}^{-1}_{\beta H_\mathrm{E}}(\sigma)\big). &(6.41)\end{aligned}$$

Inserting the above equation into the equation (6.38), we obtain

$$\begin{aligned}\mathcal{F}_{\lambda_\mathrm{f},[\lambda],\lambda_\mathrm{i}}(\sigma) &= \frac{Z_\mathrm{I}(\lambda_\mathrm{f})}{Z_\mathrm{I}(\lambda_\mathrm{i})}\mathcal{J}_{\beta H_\mathrm{E}}\Big(\mathrm{Tr}_\mathrm{IC}\Big[\rho_\mathrm{IC}(\lambda_\mathrm{f})\mathcal{M}_{[\lambda]}\big(|\lambda_\mathrm{i}\rangle_\mathrm{C}\langle\lambda_\mathrm{i}| \otimes \mathcal{J}^{-1}_{\beta H_\mathrm{E}}(\sigma)\big)\Big]\Big) &(6.42)\\ &= e^{\beta\Delta F_\mathrm{I}(\lambda_\mathrm{f},\lambda_\mathrm{i})}\mathcal{J}_{\beta H_\mathrm{E}}\Big(\mathrm{Tr}_\mathrm{IC}\Big[\rho_\mathrm{IC}(\lambda_\mathrm{f})\mathcal{M}_{[\lambda]}\big(|\lambda_\mathrm{i}\rangle_\mathrm{C}\langle\lambda_\mathrm{i}| \otimes \mathcal{J}^{-1}_{\beta H_\mathrm{E}}(\sigma)\big)\Big]\Big), &(6.43)\end{aligned}$$

where $\Delta F_\mathrm{I}(\lambda_\mathrm{f}, \lambda_\mathrm{i}) := F_\mathrm{I}(\lambda_\mathrm{f}) - F_\mathrm{I}(\lambda_\mathrm{i})$ is the difference of the Helmholtz free energies. On the other hand, from the equations (6.37) and (6.39), we obtain

$$\mathcal{R}^{\ominus}_{\tilde{\lambda}_\mathrm{f},[\tilde{\lambda}],\tilde{\lambda}_\mathrm{i}}(\sigma) = \mathrm{Tr}_\mathrm{IC}\Big[\rho_\mathrm{IC}(\lambda_\mathrm{f})\mathcal{M}_{[\lambda]}\big(|\lambda_\mathrm{i}\rangle_\mathrm{C}\langle\lambda_\mathrm{i}| \otimes \sigma\big)\Big]. \tag{6.44}$$

Combining the equations (6.43) and (6.44), we obtain

$$\mathcal{F}_{\lambda_\mathrm{f},[\lambda],\lambda_\mathrm{i}}(\sigma) = e^{\beta\Delta F_\mathrm{I}(\lambda_\mathrm{f},\lambda_\mathrm{i})}\mathcal{J}_{\beta H_\mathrm{E}} \circ \mathcal{R}^{\ominus}_{\tilde{\lambda}_\mathrm{f},[\tilde{\lambda}],\tilde{\lambda}_\mathrm{i}} \circ \mathcal{J}^{-1}_{\beta H_\mathrm{E}}(\sigma). \tag{6.45}$$

Because the equation (6.45) satisfies any initial state σ of the external system, we can rewrite the equation (6.45) as

$$\mathcal{F}_{\lambda_\mathrm{f},[\lambda],\lambda_\mathrm{i}} = e^{\beta\Delta F_\mathrm{I}(\lambda_\mathrm{f},\lambda_\mathrm{i})}\mathcal{J}_{\beta H_\mathrm{E}}\mathcal{R}^{\ominus}_{\tilde{\lambda}_\mathrm{f},[\tilde{\lambda}],\tilde{\lambda}_\mathrm{i}}\mathcal{J}^{-1}_{\beta H_\mathrm{E}}. \tag{6.46}$$

The equation (6.46) is a relation between the forward and the backward-like processes and the extension of the fluctuation relation between the forward and backward process derived in the reference [121]. In particular, when the summation $\sum_\lambda \mathcal{M}_\lambda$ of the instrument measurement $\{\, \mathcal{M}_\lambda \,\}_\lambda$ in the continuous measurement (6.31) is unital map, the equation (6.46) becomes the relation between the forward and backward continuous measurement processes.

6.3 Jarzynski equality

In this section, we derive the Jarzynski equality from the equation (6.46). We define the work extracted by the external agent E in terms of the difference between the measured energies before and after the process.

Let us denote the spectral decomposition of the Hamiltonian H_{E} by

$$H_{\mathrm{E}} = \sum_n E_n P_n, \tag{6.47}$$

where E_n and P_n are the eigenvalue of H_{E} and the corresponding projection, respectively. Because the map $\mathcal{F}_{\lambda_{\mathrm{f}},[\lambda],\lambda_{\mathrm{i}}}$ is a continuous measurement process, we can define the probability distribution of the extracted work W, the final state $|\lambda_{\mathrm{f}}\rangle$ of the control system C and the measurement recored $[\lambda]$ under the initial state $|\lambda_{\mathrm{i}}\rangle$ of the control system C by

$$P_{\mathrm{F}}(W, \lambda_{\mathrm{f}}, [\lambda]|\lambda_{\mathrm{i}}) := \sum_{n,m} \delta(W - E_m + E_n)\mathrm{Tr}\big[P^{\mathrm{E}}_m \mathcal{F}_{\lambda_{\mathrm{f}},[\lambda],\lambda_{\mathrm{i}}}\big(P^{\mathrm{E}}_n \sigma P^{\mathrm{E}}_n\big)\big], \tag{6.48}$$

where $\delta(x)$ is the delta function. In addition, the probability of the final state $|\lambda_{\mathrm{f}}\rangle$ of the control system C and the measurement recored $[\lambda]$ under the initial state $|\lambda_{\mathrm{i}}\rangle$ of the control system C is given by

$$\begin{aligned} P_{\mathrm{F}}(\lambda_{\mathrm{f}}, [\lambda]|\lambda_{\mathrm{i}}) &:= \int dW\, P_{\mathrm{F}}(W, \lambda_{\mathrm{f}}, [\lambda]|\lambda_{\mathrm{i}}) & (6.49)\\ &= \sum_{n,m} \mathrm{Tr}\big[P^{\mathrm{E}}_m \mathcal{F}_{\lambda_{\mathrm{f}},[\lambda],\lambda_{\mathrm{i}}}\big(P^{\mathrm{E}}_n \sigma P^{\mathrm{E}}_n\big)\big] & (6.50)\\ &= \mathrm{Tr}\big[\mathcal{F}_{\lambda_{\mathrm{f}},[\lambda],\lambda_{\mathrm{i}}} \circ \mathcal{P}_{H_{\mathrm{E}}}(\sigma)\big], & (6.51) \end{aligned}$$

where $\mathcal{P}_A(\bullet) := \sum_a \mathcal{P}_{A,a}(\bullet) = \sum_a P_a \bullet P_a$ with the projection P_a of the eigenvalue a of the Hermitian operator A. Because $\mathcal{P}_A$ is the trace preserving, $\mathcal{P}_{H_{\mathrm{IC}}+H_{\mathrm{E}}} = \mathcal{P}_{H_{\mathrm{IC}}} \otimes \mathcal{P}_{H_{\mathrm{E}}}$ and $\mathcal{P}_{H_{\mathrm{IC}}}$ satisfies

$$\begin{aligned} |\lambda_{\mathrm{f}}\rangle_{\mathrm{C}}\langle\lambda_{\mathrm{f}}|\mathcal{P}_{H_{\mathrm{IC}}}(A) &= \mathcal{P}_{H_{\mathrm{IC}}}\big(|\lambda_{\mathrm{f}}\rangle_{\mathrm{C}}\langle\lambda_{\mathrm{f}}|A\big), & (6.52)\\ \mathcal{P}_{H_{\mathrm{IC}}}(\rho_{\mathrm{IC}}(\lambda_{\mathrm{i}})) &= \rho_{\mathrm{IC}}(\lambda_{\mathrm{i}}) & (6.53) \end{aligned}$$

for any operator A. We thereby have

$$\begin{aligned} \mathcal{F}_{\lambda_{\mathrm{f}},[\lambda],\lambda_{\mathrm{i}}} \circ \mathcal{P}_{H_{\mathrm{E}}}(\sigma) &= \mathrm{Tr}_{\mathrm{IC}}\big[|\lambda_{\mathrm{f}}\rangle_{\mathrm{C}}\langle\lambda_{\mathrm{f}}|\mathcal{M}_{[\lambda]}\big(\rho_{\mathrm{IC}}(\lambda_{\mathrm{i}}) \otimes \mathcal{P}_{H_{\mathrm{E}}}(\sigma)\big)\big] & (6.54)\\ &= \mathrm{Tr}_{\mathrm{IC}}\big[|\lambda_{\mathrm{f}}\rangle_{\mathrm{C}}\langle\lambda_{\mathrm{f}}|\mathcal{M}_{[\lambda]} \circ \mathcal{P}_{H_{\mathrm{IC}}+H_{\mathrm{E}}}(\rho_{\mathrm{IC}}(\lambda_{\mathrm{i}}) \otimes \sigma)\big] & (6.55)\\ &= \mathrm{Tr}_{\mathrm{IC}}\big[|\lambda_{\mathrm{f}}\rangle_{\mathrm{C}}\langle\lambda_{\mathrm{f}}|\mathcal{P}_{H_{\mathrm{IC}}+H_{\mathrm{E}}} \circ \mathcal{M}_{[\lambda]}(\rho_{\mathrm{IC}}(\lambda_{\mathrm{i}}) \otimes \sigma)\big] & (6.56)\\ &= \mathcal{P}_{H_{\mathrm{E}}}\Big(\mathrm{Tr}_{\mathrm{IC}}\big[\mathcal{P}_{H_{\mathrm{IC}}}\big(|\lambda_{\mathrm{f}}\rangle_{\mathrm{C}}\langle\lambda_{\mathrm{f}}|\mathcal{M}_{[\lambda]}(\rho_{\mathrm{IC}}(\lambda_{\mathrm{i}}) \otimes \sigma)\big)\big]\Big) & (6.57)\\ &= \mathcal{P}_{H_{\mathrm{E}}} \circ \mathcal{F}_{\lambda_{\mathrm{f}},[\lambda],\lambda_{\mathrm{i}}}(\sigma), & (6.58) \end{aligned}$$

which is followed by

$$P_{\mathrm{F}}(\lambda_{\mathrm{f}}, [\lambda]|\lambda_{\mathrm{i}}) = \mathrm{Tr}\big[\mathcal{F}_{\lambda_{\mathrm{f}},[\lambda],\lambda_{\mathrm{i}}}(\sigma)\big]. \tag{6.59}$$

Using Bayes' rule, we obtain the probability distribution of the extracted work W under the measurement recored $[\lambda]$ and the initial $|\lambda_\mathrm{i}\rangle$ and final $|\lambda_\mathrm{f}\rangle$ states of the control system C as in

$$P_\mathrm{F}(W|\lambda_\mathrm{f},[\lambda],\lambda_\mathrm{i}) := \frac{P_\mathrm{F}(W,\lambda_\mathrm{f},[\lambda]|\lambda_\mathrm{i})}{P_\mathrm{F}(\lambda_\mathrm{f},[\lambda]|\lambda_\mathrm{i})}. \tag{6.60}$$

We define the conditional average by

$$\langle f(W)\rangle_{\lambda_\mathrm{f},[\lambda],\lambda_\mathrm{i}} := \int dW\, f(W) P_\mathrm{F}(W|\lambda_\mathrm{f},[\lambda],\lambda_\mathrm{i}), \tag{6.61}$$

where $f(W)$ is an arbitrary function of the extracted work W.

Let us calculate $\left\langle e^{\beta W}\right\rangle_{\lambda_\mathrm{f},[\lambda],\lambda_\mathrm{i}}$. Using the relation (6.46), we obtain

$$\mathrm{Tr}\left[P^\mathrm{E}_m \mathcal{F}_{\lambda_\mathrm{f},[\lambda],\lambda_\mathrm{i}}\left(P^\mathrm{E}_n \sigma P^\mathrm{E}_n\right)\right] = e^{\beta\Delta F_\mathrm{I}(\lambda_\mathrm{f},\lambda_\mathrm{i})}\mathrm{Tr}\left[P^\mathrm{E}_m \mathcal{J}_{\beta H_\mathrm{E}} \circ \mathcal{R}^{\ominus}_{\tilde{\lambda}_\mathrm{f},[\tilde{\lambda}],\tilde{\lambda}_\mathrm{i}} \circ \mathcal{J}^{-1}_{\beta H_\mathrm{E}}\left(P^\mathrm{E}_n \sigma P^\mathrm{E}_n\right)\right] \tag{6.62}$$

$$= e^{\beta\Delta F_\mathrm{I}(\lambda_\mathrm{f},\lambda_\mathrm{i})} e^{-\beta(E_m-E_n)}\mathrm{Tr}\left[P^\mathrm{E}_m \mathcal{R}^{\ominus}_{\tilde{\lambda}_\mathrm{f},[\tilde{\lambda}],\tilde{\lambda}_\mathrm{i}}\left(P^\mathrm{E}_n \sigma P^\mathrm{E}_n\right)\right], \tag{6.63}$$

which is followed by

$$P_\mathrm{F}(W,\lambda_\mathrm{f},[\lambda]|\lambda_\mathrm{i})$$

$$= e^{\beta\Delta F_\mathrm{I}(\lambda_\mathrm{f},\lambda_\mathrm{i})}\sum_{n,m}\delta(W-E_m+E_n)e^{-\beta(E_m-E_n)}\mathrm{Tr}\left[P^\mathrm{E}_m \mathcal{R}^{\ominus}_{\tilde{\lambda}_\mathrm{f},[\tilde{\lambda}],\tilde{\lambda}_\mathrm{i}}\left(P^\mathrm{E}_n \sigma P^\mathrm{E}_n\right)\right] \tag{6.64}$$

$$= e^{\beta\Delta F_\mathrm{I}(\lambda_\mathrm{f},\lambda_\mathrm{i})}e^{-\beta W}\sum_{n,m}\delta(W-E_m+E_n)\mathrm{Tr}\left[P^\mathrm{E}_m \mathcal{R}^{\ominus}_{\tilde{\lambda}_\mathrm{f},[\tilde{\lambda}],\tilde{\lambda}_\mathrm{i}}\left(P^\mathrm{E}_n \sigma P^\mathrm{E}_n\right)\right]. \tag{6.65}$$

Therefor, we obtain

$$\left\langle e^{\beta W}\right\rangle_{\lambda_\mathrm{f},[\lambda],\lambda_\mathrm{i}} = e^{\beta\Delta F_\mathrm{I}(\lambda_\mathrm{f},\lambda_\mathrm{i})}\frac{\mathrm{Tr}\left[\mathcal{R}^{\ominus}_{\tilde{\lambda}_\mathrm{f},[\tilde{\lambda}],\tilde{\lambda}_\mathrm{i}} \circ \mathcal{P}_{H_\mathrm{E}}(\sigma)\right]}{P_\mathrm{F}(\lambda_\mathrm{f},[\lambda]|\lambda_\mathrm{i})}. \tag{6.66}$$

Similarly to the equation (6.58), we obtain

$$\mathcal{R}^{\ominus}_{\tilde{\lambda}_\mathrm{f},[\tilde{\lambda}],\tilde{\lambda}_\mathrm{i}}\mathcal{P}_{H_\mathrm{E}} = \mathcal{P}_{H_\mathrm{E}}\mathcal{R}^{\ominus}_{\tilde{\lambda}_\mathrm{f},[\tilde{\lambda}],\tilde{\lambda}_\mathrm{i}}, \tag{6.67}$$

and thereby obtain

$$\left\langle e^{\beta W}\right\rangle_{\lambda_\mathrm{f},[\lambda],\lambda_\mathrm{i}} = \gamma_{\lambda_\mathrm{i},[\lambda],\lambda_\mathrm{f}}\, e^{\beta\Delta F_\mathrm{I}(\lambda_\mathrm{f},\lambda_\mathrm{i})} \tag{6.68}$$

with

$$\gamma_{\lambda_\mathrm{i},[\lambda],\lambda_\mathrm{f}} := \frac{\mathrm{Tr}\left[\mathcal{R}^{\ominus}_{\tilde{\lambda}_\mathrm{f},[\tilde{\lambda}],\tilde{\lambda}_\mathrm{i}}(\sigma)\right]}{P_\mathrm{F}(\lambda_\mathrm{f},[\lambda]|\lambda_\mathrm{i})}. \tag{6.69}$$

This is the quantum Jarzynski equality under the continuously monitored control parameter.

Note that the equation (6.68) focuses on the external agent E, not the composite system IC; the coefficient $\gamma_{\lambda_\mathrm{i},[\lambda],\lambda_\mathrm{f}}$ is given from the continuous measurement in the external agent E. On the other hand, the quantum Jarzynski equality in the chapter 5 focuses on the composite system IC. However, we can rewrite the coefficient (6.69) as the coefficient given from the continuous measurement in measurement of the composite system IC as follows.

Let us define the continuous measurement of the composite system IC by

$$\mathcal{K}_{[\lambda]}(\rho) := \mathrm{Tr}_{\mathrm{E}}\big[\mathcal{M}_{[\lambda]}(\rho \otimes \sigma)\big], \tag{6.70}$$

where ρ is an arbitrary state of the composite system IC and Tr_{E} is the partial trace over the external agent E. Then, we obtain

$$\begin{aligned} P_{\mathrm{F}}(\lambda_{\mathrm{f}}, [\lambda]|\lambda_{\mathrm{i}}) &= \mathrm{Tr}\big[\mathcal{F}_{\lambda_{\mathrm{f}},[\lambda],\lambda_{\mathrm{i}}}(\sigma)\big] & (6.71)\\ &= \mathrm{Tr}\Big[|\lambda_{\mathrm{f}}\rangle_{\mathrm{C}}\langle\lambda_{\mathrm{f}}|\mathcal{M}_{[\lambda]}(\rho_{\mathrm{IC}}(\lambda_{\mathrm{i}}) \otimes \sigma)\Big] & (6.72)\\ &= \mathrm{Tr}\Big[|\lambda_{\mathrm{f}}\rangle_{\mathrm{C}}\langle\lambda_{\mathrm{f}}|\mathcal{K}_{[\lambda]}(\rho_{\mathrm{IC}}(\lambda_{\mathrm{i}}))\Big]. & (6.73) \end{aligned}$$

On the other hand, using the equation (6.44), the numerator of the coefficient (6.69) is rewritten by

$$\begin{aligned} \mathrm{Tr}\Big[\mathcal{R}^{\ominus}_{\tilde{\lambda}_{\mathrm{f}},[\tilde{\lambda}],\tilde{\lambda}_{\mathrm{i}}}(\sigma)\Big] &= \mathrm{Tr}\Big[\rho_{\mathrm{IC}}(\lambda_{\mathrm{f}})\mathcal{M}_{[\lambda]}\big(|\lambda_{\mathrm{i}}\rangle_{\mathrm{C}}\langle\lambda_{\mathrm{i}}| \otimes \sigma\big)\Big] & (6.74)\\ &= \mathrm{Tr}\Big[\rho_{\mathrm{IC}}(\lambda_{\mathrm{f}})\mathcal{K}_{[\lambda]}\big(|\lambda_{\mathrm{i}}\rangle_{\mathrm{C}}\langle\lambda_{\mathrm{i}}|\big)\Big]. & (6.75) \end{aligned}$$

Therefore, we obtain the coefficient $\gamma_{\lambda_{\mathrm{i}},[\lambda],\lambda_{\mathrm{f}}}$ given from the continuous measurement $\mathcal{K}_{[\lambda]}$ of the composite system IC.

Applying the Jensen inequality $\langle e^{f}\rangle \geq e^{\langle f\rangle}$ to the quantum Jarzynski equality (6.68), we obtain

$$\langle W\rangle_{\lambda_{\mathrm{f}},[\lambda],\lambda_{\mathrm{i}}} \leq -\Delta F_{\mathrm{I}}(\lambda_{\mathrm{f}}, \lambda_{\mathrm{i}}) + \beta^{-1}\log\gamma_{\lambda_{\mathrm{i}},[\lambda],\lambda_{\mathrm{f}}}. \tag{6.76}$$

This inequality is the second law under the continuously monitored control parameter.

Similarly to the chapter 5, the difference between the conventional approach and the new formulation of the work extraction is given by the coefficient $\gamma_{\lambda_{\mathrm{i}},[\lambda],\lambda_{\mathrm{f}}}$. Obviously, the coefficient $\gamma_{\lambda_{\mathrm{i}},[\lambda],\lambda_{\mathrm{f}}}$ is not generally equal to unity, and does not generally become unity when the time evolution is a unital map. In particular, when the coefficient $\gamma_{\lambda_{\mathrm{i}},[\lambda],\lambda_{\mathrm{f}}}$ is greater than unity, the equation (6.76) permits the extracted work to break the second law. However, as you will see in the next section, we show the fact that the probability of the measurement record breaking the second law is very small.

6.4 Relation between control parameter and second law

Let us show the relation between the probability of the measurement record and the second law.

Translating the equation (6.76), we obtain

$$P_{\mathrm{F}}(\lambda_{\mathrm{f}}, [\lambda]|\lambda_{\mathrm{i}}) \leq \mathrm{Tr}\Big[\mathcal{R}^{\ominus}_{\tilde{\lambda}_{\mathrm{f}},[\tilde{\lambda}],\tilde{\lambda}_{\mathrm{i}}}(\sigma)\Big]e^{-\beta\left(\langle W\rangle_{\lambda_{\mathrm{f}},[\lambda],\lambda_{\mathrm{i}}}+\Delta F_{\mathrm{I}}(\lambda_{\mathrm{f}},\lambda_{\mathrm{i}})\right)}. \tag{6.77}$$

Using the equation (6.75) and $\mathrm{Tr}\big[\mathcal{K}_{[\lambda]}(\rho)\big] \leq 1$ for an arbitrary state ρ of the composite system IC, we obtain

$$\begin{aligned}
\mathrm{Tr}\Big[\mathcal{R}^{\ominus}_{\tilde{\lambda}_\mathrm{f},[\tilde{\lambda}],\tilde{\lambda}_\mathrm{i}}(\sigma)\Big] &= \mathrm{Tr}\Big[\rho_\mathrm{IC}(\lambda_\mathrm{f})\mathcal{K}_{[\lambda]}\big(|\lambda_\mathrm{i}\rangle_\mathrm{C}\langle\lambda_\mathrm{i}|\big)\Big] && (6.78)\\
&\leq p_\mathrm{max}(\lambda_\mathrm{f})\mathrm{Tr}\Big[|\lambda_\mathrm{f}\rangle_\mathrm{C}\langle\lambda_\mathrm{f}|\mathcal{K}_{[\lambda]}\big(I_\mathrm{I}\otimes|\lambda_\mathrm{i}\rangle_\mathrm{C}\langle\lambda_\mathrm{i}|\big)\Big] && (6.79)\\
&\leq p_\mathrm{max}(\lambda_\mathrm{f})\mathrm{Tr}\Big[\mathcal{K}_{[\lambda]}\big(I_\mathrm{I}\otimes|\lambda_\mathrm{i}\rangle_\mathrm{C}\langle\lambda_\mathrm{i}|\big)\Big] && (6.80)\\
&\leq D_\mathrm{I}\, p_\mathrm{max}(\lambda_\mathrm{f}), && (6.81)
\end{aligned}$$

where I_I is the identity operator on the internal system I, D_I is the dimensional of the internal system I and $p_\mathrm{max}(\lambda)$ is the maximal eigenvalue of $\rho_\mathrm{IC}(\lambda)$. Inserting the equation (6.81) into the equation (6.77), we obtain

$$P_\mathrm{F}(\lambda_\mathrm{f},[\lambda]|\lambda_\mathrm{i}) \leq p_\mathrm{max}(\lambda_\mathrm{f})e^{-\beta\left(\langle W\rangle_{\lambda_\mathrm{f},[\lambda],\lambda_\mathrm{i}}+\Delta F_\mathrm{I}(\lambda_\mathrm{f},\lambda_\mathrm{i})-\beta^{-1}\log D_\mathrm{S}\right)}, \tag{6.82}$$

As we can see in the equation (6.82), the probability of the measurement record breaking the upper limit of the second law of information thermodynamics

$$\langle W\rangle \leq -\Delta F_\mathrm{I} + \beta^{-1}\log D_\mathrm{I} \tag{6.83}$$

exponentially decreases.

In particular, if the non-selective continuous measurement $\mathcal{K} := \int\mathcal{D}[\lambda]\mathcal{K}_{[\lambda]}$ of the composite system IC is a unital map, we obtain

$$\mathcal{K}_{[\lambda]}\big(I_\mathrm{I}\otimes|\lambda_\mathrm{i}\rangle_\mathrm{C}\langle\lambda_\mathrm{i}|\big) \leq \mathcal{K}\big(I_\mathrm{I}\otimes|\lambda_\mathrm{i}\rangle_\mathrm{C}\langle\lambda_\mathrm{i}|\big) \leq \mathcal{K}(I_\mathrm{I}\otimes I_\mathrm{C}) = I_\mathrm{I}\otimes I_\mathrm{C}, \tag{6.84}$$

where I_C is the identity operator on the control system C. Then, using the equation (6.75), we obtain

$$\mathrm{Tr}\Big[\mathcal{R}^{\ominus}_{\tilde{\lambda}_\mathrm{f},[\tilde{\lambda}],\tilde{\lambda}_\mathrm{i}}(\sigma)\Big] \leq \mathrm{Tr}[\rho_\mathrm{IC}(\lambda_\mathrm{f})(I_\mathrm{I}\otimes I_\mathrm{C})] = 1, \tag{6.85}$$

and thereby obtain

$$P_\mathrm{F}(\lambda_\mathrm{f},[\lambda]|\lambda_\mathrm{i}) \leq e^{-\beta\left(\langle W\rangle_{\lambda_\mathrm{f},[\lambda],\lambda_\mathrm{i}}+\Delta F_\mathrm{I}(\lambda_\mathrm{f},\lambda_\mathrm{i})\right)}. \tag{6.86}$$

As we can see in the above equation, the probability of the measurement record breaking the upper limit of the second law of thermodynamics exponentially decreases.

6.5 Summary of this chapter

In this chapter, we introduced the continuous measurement of the control system in order to compare the conventional approach and the new formulation of the work extraction under the closer situation.

In the section 6.1, we described the time reversal introduced by Åberg [121] and the time reversal of continuous measurement to derive another quantum version of the Jarzynski equality. From consideration of the time reversal of continuous measurement, we introduced a backward-like continuous measurement, whose measurement record is given by the reverse order of a forward measurement record but which does not satisfies the properties of quantum measurement.

In order to derive the quantum version of the Jarzynski equality, we first considered the relation between the forward and backward-like continuous measurements in the section 6.2. As a result, we obtained the fluctuation relation between the forward and backward-like continuous measurements of the equation (6.46). This relation is an extension of the fluctuation relation between the forward and backward processes, which was derived in the reference [121].

Using the fluctuation relation in the section 6.2, we derived the quantum version of the Jarzynski equality under the continuous measurement. As a result, we obtained the coefficient $\gamma_{\lambda_\mathrm{i},[\lambda],\lambda_\mathrm{f}}$ as the difference from the conventional derivation of the Jarzynski equality. Similarly to the quantum version of the Jarzynski equality in the chapter 5, the coefficient $\gamma_{\lambda_\mathrm{i},[\lambda],\lambda_\mathrm{f}}$ is not generally equal to unity. In other words, the influence of the work extraction as the measurement process is not erased by the continuous measurement of the control system C.

The coefficient $\gamma_{\lambda_\mathrm{i},[\lambda],\lambda_\mathrm{f}}$ can be greater than unity, in which case the second law is violated. However, we can find that the measurement record violating the second law happens only with a small probability, and hence the second law is not violated in the expectation over all the measurement records. In other words, we may experimentally detect the difference between the conventional approach and the new formulation of the work extraction with a small but finite probability.

Chapter 7

Conclusion

In the present thesis, we derived quantum versions of the Jarzynski equality under the two situations in the chapters 5 and 6.

In the chapter 5, we first showed that the variance of the energy obtained by the external agent diverges when the time evolution of the thermodynamic system is approximated to a unitary one. This result is a good counterexample of the conventional approach using a time-dependent Hamiltonian. This counterexample revealed that the work extraction of the conventional approach is unsuitable for quantum thermodynamics. We claim that the work extraction from a microscope quantum system should be described as a quantum measurement process in the chapter 4. We have applied the new approach to the quantum Jarzynski equality. Our derivation of the quantum Jarzynski equality is essentially different from the conventional derivation; our derivation correctly contains information about the fluctuation of the actual work, namely, the energy gain of the external agent. The difference between the conventional and our derivation of the quantum Jarzynski equality appears as the coefficient γ in the cyclic process and the coefficient $\gamma_{\lambda_\mathrm{i}\to\lambda_\mathrm{f}}$ in the non-cyclic process. In the case of the conventional derivations in the cyclic and non-cyclic processes, these coefficients γ and $\gamma_{\lambda_\mathrm{i}\to\lambda_\mathrm{f}}$ are always equal to unity, but those in the case of our derivation are not generally equal to unity. This differences are caused by describing the work extraction in terms of the quantum measurement process. The coefficient γ in the cyclic process is equal to unity when the work extraction is the “natural” thermodynamic process, which satisfies the second law of thermodynamic for an arbitrary operation. Hence, the condition $\gamma \neq 1$ is caused by the feedback effect of quantum measurement. On the other hand, the coefficient $\gamma_{\lambda_\mathrm{i}\to\lambda_\mathrm{f}}$ in the non-cyclic process is not generally equal to unity even when the work extraction is the “natural” thermodynamic process and widely fluctuates around unity, which we exemplified for a simple model in the section 5.3. This comes from the irreversibility of the control system. We expect to detect this fluctuation experimentally and to provide evidence for the new approach.

In the chapter 6, we derived the quantum Jarzynski equality under the continuously monitored control parameter and the relation between the continuously monitored control parameter and the second law of thermodynamics. Because the quantum Jarzynski equality in the chapter 6 is unclear as to how the microscope quantum system is operated by the external agent, we have resolved it by observing the control parameter continuously. Similarly to the quantum version of the Jarzynski equality in the chapter 5, we obtain the coefficient $\gamma_{\lambda_\mathrm{i},[\lambda],\lambda_\mathrm{f}}$, which is not generally equal to unity, as the difference from the conventional derivation.. Hence, the influence of the work extraction in terms of the measurement process is not erased by the continuously monitored control parameter. The coefficient $\gamma_{\lambda_{\mathrm{i}},[\lambda],\lambda_{\mathrm{f}}}$ can be greater than unity, in which case the second law is violated. On the other hand, we find that the measurement record violating the second law happens only with a small probability. Hence, the second law is not violated in the expectation over all the measurement records. In other wards, we may experimentally detect the difference from the conventional derivation with a small but finite probability.

Let us finally summarize two tasks remaining to be resolved. In the chapters 5 and 6, we have assumed that the measurement process of the work extraction can measure the energy loss of the internal system without errors; in other words, it can convert all of the energy loss into the work. However, since the actual external agent is a thermodynamics system, the energy transfer may be separated into the work and the heat. The work extraction process corresponding to this should be an incomplete process in which the extracted work is not equal to the energy loss. In is an important issue to be resolved.

Moreover, in the chapter 6, we have assumed that the continuous measurement of the control parameter preserves the energy of the total system. However, the actual continuously monitoring of an observable generally gives rise to the energy exchange between the measurement device and the monitored system. The continuous measurement should take into account the energy change by the monitoring.

Appendix A

Adjoint of CP map

An adjoint map $\mathcal{K}^\dagger$ of a completely positive (CP) map $\mathcal{K}$ is defined in

$$\mathrm{Tr}\left[\mathcal{K}^\dagger(B)A\right] = \mathrm{Tr}[B\mathcal{K}(A)], \tag{A.1}$$

where A and B are arbitrary bounded operators. For the Kraus representation $\mathcal{K}(A) = \sum_n K_n A K_n^\dagger$, we have

$$\mathcal{K}^\dagger(A) = \sum_n K_n^\dagger A K_n. \tag{A.2}$$

Therefore, the adjoint $\mathcal{K}^\dagger$ is also a CP map. Note that the adjoint of a trace preserving (TP) CP map does not generally preserve the trace, because $\mathrm{Tr}\left[\mathcal{K}^\dagger(B)\right] = \mathrm{Tr}[B\mathcal{K}(I)] \neq \mathrm{Tr}[B]$ for any operator B, where I is the identity operator. The adjoint of a TPCP map $\mathcal{K}$ preserves the trace if and only if the TPCP map $\mathcal{K}$ is a unital map, which satisfies $\mathcal{K}(I) = I$.

Let $\mathcal{K}$ and $\mathcal{L}$ denote CP maps. Then, the adjoint of $\mathcal{K}\mathcal{L}$ is equal to $\mathcal{L}^\dagger\mathcal{K}^\dagger$, because

$$\mathrm{Tr}\left[(\mathcal{K}\mathcal{L})^\dagger(B)A\right] = \mathrm{Tr}[B(\mathcal{K}\mathcal{L})(A)] = \mathrm{Tr}\left[\mathcal{K}^\dagger(B)\mathcal{L}(A)\right] = \mathrm{Tr}\left[\mathcal{L}^\dagger\mathcal{K}^\dagger(B)A\right]. \tag{A.3}$$

We now consider the adjoint using the reference system. Let U denotes a unitary operator on the system composed by a system S of interest and a reference system R. Then, the CP map can be given by

$$\mathcal{K}(A) := \mathrm{Tr}_{\mathrm{R}}\left[(I_{\mathrm{S}} \otimes P_{\mathrm{R}})U(A \otimes Q_{\mathrm{R}})U^\dagger\right], \tag{A.4}$$

where P_{R} and Q_{R} are positive operators on the reference system R, I_{S} is the identity operator on the system S and Tr_{R} denotes the partial trace over the reference system R. Using the cyclic property of the trace, we obtain

$$\begin{aligned}
\mathrm{Tr}[B\mathcal{K}(A)] &= \mathrm{Tr}\left[B\,\mathrm{Tr}_{\mathrm{R}}\left[(I_{\mathrm{S}} \otimes P_{\mathrm{R}})U(A \otimes Q_{\mathrm{R}})U^\dagger\right]\right] && \text{(A.5)}\\
&= \mathrm{Tr}\left[(B \otimes P_{\mathrm{R}})U(A \otimes Q_{\mathrm{R}})U^\dagger\right] && \text{(A.6)}\\
&= \mathrm{Tr}\left[U^\dagger(B \otimes Q_{\mathrm{R}})U(A \otimes Q_{\mathrm{R}})\right] && \text{(A.7)}\\
&= \mathrm{Tr}\left[\mathrm{Tr}_{\mathrm{R}}\left[(I_{\mathrm{S}} \otimes Q_{\mathrm{R}})U^\dagger(B \otimes P_{\mathrm{R}})U\right]A\right]. && \text{(A.8)}
\end{aligned}$$

Therefore, the adjoint of $\mathcal{K}$ is represented by [121]

$$\mathcal{K}^\dagger(A) = \mathrm{Tr}_{\mathrm{R}}\left[(I_{\mathrm{S}} \otimes Q_{\mathrm{R}})U^\dagger(A \otimes P_{\mathrm{R}})U\right]. \tag{A.9}$$

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