Doctoral Dissertation

Application of the Generalized Work Relation for an N-level Quantum System

March 2015

Major in Mathematical Science
Graduate School of Science and Engineering
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Abstract

We generalized the maximum work formulation of the second law for a nonequilibrium initial state. This generalization allows us to find the maximum work that can be gained from a nonequilibrium initial state. We are able to consider isolated systems as well as those coupled to heat reservoirs, undergoing both adiabatic and isothermal transitions.

The derivation is based on the information geometry. The maximum work formulation is generalized as a relation between the work and a relative entropy with an effective temperature. The relative entropy, also known as the Kullback–Leibler divergence, is always positive and gives a "distance" between the nonequilibrium initial distribution and the canonical distribution.

For a finite Hamiltonian system without a heat reservoir, the effective temperature is determined by an isentropic condition. The maximum work is realized in two successive processes: an instantaneous stabilization of the nonequilibrium initial distribution and an isentropic process. When the system is coupled to a large heat reservoir, the effective temperature is the temperature of the heat reservoir. From the generalized second law, the maximum work is realized in two successive processes: an instantaneous stabilization and a quasi-static isothermal process.

In this thesis, we explicitly show how the maximum work is realized in the limit of instantaneous stabilization in a finite quantum system. Instantaneous stabilization does not appear in traditional thermodynamics. We introduced this process in order to extract the maximum work from the nonequilibrium initial state. It prevents spontaneous relaxation such as free expansion in a gas system. Since it is an ideal instantaneous process, its realizability is a crucial problem we must consider.

We consider a finite quantum system with a Hamiltonian that has a time dependence associated with an external cyclic operation. The first step in extracting work from a nonequilibrium initial state is to stop its time evolution. This may be accomplished by changing the initial Hamiltonian to an effective Hamiltonian for which the nonequilibrium initial state is a stable canonical distribution. After the stabilization, we performed an isentropic process which changes the effective Hamiltonian to the final Hamiltonian. We show how the maximum work is realized in the limit of instantaneous stabilization in an exactly solvable two–level system.

We confirm that the generalized work relation is consistent with known results. Several authors showed the validity of the second law for a passive initial state in an N–level system. Hatsopoulos–Gyftopoulos and Allahverdyan–Balian–Nieuwenhuizen obtained the maximum work from a non-passive initial state. Our result is completely consistent with their results.

We show how to extract the maximum work for a process that includes a crossing of adiabatic energy levels. Work extracted from a thermally isolated equilibrium system is maximized for quasi-static realization of a given process. Allahverdyan and Nieuwenhuizen rigorously showed that this principle can be violated for crossings of adiabatic energy levels. Therefore, we give a non-quasi-static process that maximizes work extraction when there is a level crossing.

Finally we propose an efficient quantum feedback control in a symmetric two–level quantum system connected to an energy source. For the symmetric two–level quantum system we may skip the restoration process. After re-excitation by the energy source, we repeat the instantaneous stabilization. Since a real stabilization is an almost instantaneous process, we can control the system even though it is coupled to an energy source. The minimum period is determined by a re-excitation time, such as the relaxation time Since our argument is not restricted within thermodynamics, we can choose any energy source, such as the light from sun, to make the re-excitation time much shorter. We expect our efficient quantum process plays an important role in a quantum dot solar cell.

Acknowledgement

My heartfelt appreciation goes to Professor Hiroshi Hasegawa who offered continuing support and constant encouragement. Without his guidance and persistent help this dissertation would not have been possible. Special thanks go to Professor Toshio Horiuchi, Professor Katsunori Shimomura, and Professor Shoichi Fujima whose comments were invaluable. I would also like to express my thanks to Dr. Kazuma Takara and Dr. Naoya Sato who gave me insightful comments and suggestions. Finaly, I owe my deepest gratitude to my family for their moral support and warm encouragement.

Contents

Chapter 1

Introduction

1.1 Background

The second law of thermodynamics is the central law of nature[1]. When a system is in equilibrium and within an isothermal condition, the Kelvin principle, one representation of the second law, is

$$W^{\mathrm{cycle}} \geq 0 \tag{1.1}$$

where W^{cycle} is work done on the system by an external cyclic operation. The second law asserts the impossibility of perpetual motion of the second kind.

Approximately two decades ago, two important theorems of nonequilibrium statistical mechanics, the fluctuation theorem[2] and Jarzynski work relation[3, 4], were rigorously proved. From these theorems, the maximum work formulation of the second law is exactly proved

$$< W^{\mathrm{cycle}} | \rho_{\mathrm{can},0}(\beta) > \geq 0 \tag{1.2}$$

where $\rho_{\mathrm{can},0}(\beta)$ is the initial canonical distribution of the system with the inverse of the temperature β and $< \bullet | \rho >$ is the expectation value integrated over a probability density ρ. The maximum work formulation of the second law is valid for the expectation value. Therefore, W^{cycle} can be negative for rare cases within finite systems as suspected by Evans-Morriss-Cohen [2]. After the proposals of these theorems, the second law was refreshed in relation with the information theory [5-12].

Recently, the maximum work formulation of the second law was generalized for a nonequilibrium initial state [13-18]. Work on the system by an external cyclic operation for a nonequilibrium initial state is bounded from below:

$$< W^{\mathrm{cycle}} | \rho_0 > \geq -\beta^{-1} D[\rho_0 || \rho_{\mathrm{can},0}(\beta)] \tag{1.3}$$

where the relative entropy (Kullback –Leibler divergence) is defined as [19]

$$D[\rho_A || \rho_B] = < \log \frac{\rho_A}{\rho_B} | \rho_A > \tag{1.4}$$

The relative entropy means the “distance” between two probability densities in the information geometry [20]. It is always positive and vanishes only for

$\rho_A = \rho_B$. In the generalization of the maximum work formulation, the relative entropy, the “distance” between the initial probability density and the initial canonical distribution, indicates the initial “nonequilibriumness”. Therefore, the generalized second law returns to the original second law for the initial equilibrium state.

The generalized second law is a universal law. It is rigorously derived from only fundamental properties of Hamiltonian dynamics (conservation of the Gibbs-Shannon entropy) and information geometry (non-negativity of the relative entropy)[20, 21]. It is applicable to a thermally isolated small classical/quantum Hamiltonian system even outside the realm of thermodynamics. In this sense the second law becomes universal parallel to the first law, which is the universal law of energy conservation.

The temperature cannot be defined for a finite isolated system. For a finite isolated system, the temperature β^{-1} in Eq.(1.3) should be replaced by an effective one $\tilde{\beta}^{-1}$ which is determined by the isentropic condition,

$$S_{\mathrm{can},0}(\tilde{\beta}) = S_0 \tag{1.5}$$

where the entropy for the canonical distribution with the effective temperature,

$$S_{\mathrm{can},0}(\tilde{\beta}) = - < \log \rho_{\mathrm{can},0}(\tilde{\beta}) | \rho_{\mathrm{can},0}(\tilde{\beta}) > \tag{1.6}$$

and the initial entropy,

$$S_0 = - < \log \rho_0 | \rho_0 > \tag{1.7}$$

The generalized second law gives a fundamental relation between energy (the maximum work) and information (the relative entropy). It is a generalization of the Landauer principle [22-27] and reduces it for a quantum system of one bit memory in a thermal bath. The energy corresponding to an unit of information is given by the effective temperature for a finite bath.

In this thesis, we consider a process to gain the maximum work from a nonequilibrium initial state. To gain maximum work from a non-equilibrium initial state, we have to avoid dissipation. To prevent spontaneous relaxation such as free expansion of gas, the initial Hamiltonian should be instantaneously changed at the beginning of the process so that the initial state is a canonical distribution for the changed Hamiltonian. This canonical distribution can evolve to the final canonical distribution in a process that is dissipationless. The final Hamiltonian should be the initial Hamiltonian for a cyclic operation.

We consider a finite quantum system: the N–level system. Its Hamiltonian has a time dependent parameter $\theta(t)$ associated with an external cyclic operation. The first step in extracting work from a nonequilibrium initial state is to stop its time evolution. This may be accomplished by changing the initial Hamiltonian to an effective Hamiltonian for which the nonequilibrium initial state is a stable canonical distribution. After the stabilization, we perform an isentropic process that changes the effective Hamiltonian to the final Hamiltonian. We show how the maximum work is realized in the limit of instantaneous stabilization in an exactly solvable two–level system. Since the process of instantaneous stabilization does not appear in traditional thermodynamics, its realizability is a problem we must consider.

The time evolution of an N–level system is quasi-periodic because the level spacings are generally finite. An N–level system is not a thermodynamic system; however it is mathematically very interesting. Lenard, Pusz–Woronowicz, Tasaki, and Allahverdyan–Nieuwenhuizen [28-31] rigorously derived the second law for an initial passive state. Furthermore, Hatsopoulos–Gyftopoulos, and Allahverdyan–Balian–Nieuwenhuizen, [32, 33]. generalized the second law for a non-passive initial state. Their arguments are based on the majorization theory for N–dimensional vector space. For a non-passive initial state, we obtain the maximum work that is completely consistent with their results.

Allahverdyan–Nieuwenhuizen also discussed the maximum work for a process that includes a crossing of adiabatic energy levels [34]. Work extracted from a thermally isolated equilibrium system is maximized for quasi-static realization of a given process. Allahverdyan–Nieuwenhuizen rigorously showed that this principle can be violated for a crossing of adiabatic energy levels. Therefore, we give a non-static process including an instantaneous stabilization that maximizes work extraction when there is a level crossing.

We finally consider a more realistic system: a two–level system connected to an energy source. We proposed an efficient quantum feedback control [27, 35] in a symmetric two–level system. We expect that our efficient quantum process plays an important role in a quantum dot solar cell.

1.2 Outlines

In Chapter 2, we consider a classical Hamiltonian system that is thermally isolated. The maximum work formulation of the second law is rigorously proved for the initial equilibrium state. When the total system is divided into two, system and heat reservoir, the maximum work formulation is extended for an isothermal process. We generalize the maximum work formulation for a nonequilibrium initial state. This generalization is extended for a transition between nonequilibrium states. In Chapter 3, we consider an N–level quantum system. A periodic operation to gain the maximum work from a nonequilibrium initial state is explicitly shown in an exactly solvable two–level system. The periodic operation consists of an instantaneous stabilization and an isentropic restoration is applied in the case of level crossing. These arguments are extended to an N–level system in which a passive state plays as the role of the canonical state. Finally we consider a two–level system connected to an energy source. An efficient quantum feedback control is proposed. In Chapter 4, we give conclusion and remarks.

This thesis is based on the following three papers of our group:

1. Generalization of the second law for a nonequilibrium initial state
   H.-H. Hasegawa, J. Ishikawa, K. Takara, and D.J. Driebe
   Physics Letters A 374 (2010) 1001-1004.
2. Generalization of the second law for a transition between
   nonequilibrium states
   K. Takara, H.-H. Hasegawa, and D.J. Driebe
   Physics Letters A 375 (2010) 88-92.
3. Application of the Generalized Work Relation for an N-level Quantum
   System
   J. Ishikawa, K. Takara, H.-H. Hasegawa and D. J. Driebe
   Entropy 16 (2014) 3471-3481.

Many parts of this thesis are quoted from these papers without explicit citation.

Chapter 2

The Generalized Second Law

In this chapter, we generalize the maximum work formulation of the second law for a transition between initial and final nonequilibium states. First, we consider a thermally isolated total system. For an equilibrium initial state, we derive the maximum work formulation in an adiabatic process. When the total system is divided into an operated system and a huge reservoir, the maximum work formulation is reconsidered in an isothermal process. Then, we generalize the maximum work formulation for a nonequilibrium initial state. When we have information about the nonequilibrium final state, we can generalize the maximum work formulation for a transition between the initial and final nonequilibium states.

Our arguments are based on the microscopic Hamiltonian dynamics and information geometry. We derive the generalized second law for classical Hamiltonian dynamics in this chapter. The derivation for quantum mechanics [36] is shown in Appendix B.

2.1 System

We consider a Hamiltonian system that is thermally isolated. The total system consists of a system we operate on and a reservoir. They are coupled to each other. The total Hamiltonian is a sum of three Hamiltonians, $H^{(\mathrm{S})}(x, a(t))$, $H^{(\mathrm{R})}(y)$ and the interaction between them, $H^{(\mathrm{I})}(x, y)$, as

$$H(r, \theta(t)) = H^{(\mathrm{S})}(x, \theta(t)) + H^{(\mathrm{R})}(y) + H^{(\mathrm{I})}(x, y) \tag{2.1}$$

where $r = (x, y) \in \Gamma$ is a phase space point of the total system. A point, x (y), is included in a phase space $\Gamma^{(\mathrm{S})}$ ($\Gamma^{(\mathrm{R})}$). The phase space of the total system is written as $\Gamma = \Gamma^{(\mathrm{S})} \times \Gamma^{(\mathrm{R})}$. $\theta(t)$ is a time-dependent parameter of the Hamiltonian of the system. $\theta(t)$ follows a given protocol associated with external operations to the system. We represent a function in the system (reservoir) with superscript, (S)((R)). We prepare a separable nonequilibrium initial probability density at the beginning $t = 0$; $\rho(r, 0) = \rho^{(\mathrm{S})}(x, 0)\rho^{(\mathrm{R})}(y, 0)$. We put them in contact for intermediate times ($0 < t < T$) then we separate them at the end

$t = T$. It is assumed that the interaction Hamiltonian is negligible for both the beginning and end.

The time evolution of the probability density of the total system is governed by Liouville equation as

$$\mathrm{i}\frac{\partial \rho(r,t)}{\partial t} = L(t)\rho(r,t) \tag{2.2}$$

where $L(t)$ is the Liouvillian corresponding to the Hamiltonian $H(r, \theta(t))$. Hereafter, we abbreviate $H_t(r) = H(r, \theta(t))$ and $\rho_t(r) = \rho(r,t)$ for convenience.

2.2 Work equality in information geometry

In this section, we show that a work in Hamiltonian dynamics is rewritten as a difference between the initial and final relative entropies (divergences) in information geometry.

In the thermally isolated Hamiltonian system, the work done on the system is given as the difference between the initial and final total energies,

$$< W|\rho_0 > \equiv < H_T|\rho_T > - < H_0|\rho_0 > \tag{2.3}$$

where the bra-ket notation is defined as

$$< f_t|\rho_t > \equiv \int_\Gamma f_t(r)\rho_t(r)dr \tag{2.4}$$

is an expectation value of a physical quantity f at time t. The probability density at time t is written as

$$\rho_t = \mathrm{U}^t\rho_0 = \mathrm{T}\exp[-i\int_0^t L(t')dt']\rho_0 \tag{2.5}$$

where T is the well-known time ordered product. Note that the time evolution operator is an unitary operator so that the Gibbs-Shannon entropy is conserved. Hereafter, we abbreviate $W =< W|\rho_0 >$ and $E_t =< H_t|\rho_t >$ for convenience. The canonical distribution at time t with temperature α^{-1} is defined as

$$\rho_{\mathrm{can},t}(\alpha) = \exp[\alpha\{F_t(\alpha) - H_t\}] \tag{2.6}$$

where the Boltzmann constant was chosen as unity. Since our temperature includes the Boltzmann constant, the dimension of our temperature is energy. The free energy is defined as a normalization factor in the canonical distribution,

$$F_t(\alpha) = -\alpha^{-1}\log\left[\int_\Gamma \exp[-\alpha H_t(r)]dr\right] \tag{2.7}$$

Our derivation of the maximum work formulation is based on fundamental properties of Hamiltonian dynamics and information geometry: conservation of the Gibbs-Shannon entropy under Hamiltonian dynamics and non-negativity of the relative entropy (Kullback-Leibler divergence). The proofs of the non-negativity of the Kullback-Leibler divergence [37] is given in Appendix A.

The Gibbs-Shannon entropy is defined as

$$S_t \equiv - < \log\rho_t|\rho_t > . \tag{2.8}$$

Since the time evolution operator is a unitary operator,

$$S_T = S_0 \tag{2.9}$$

The relative entropy (Kullbac–Leibler divergence) between a probability density of the system and the canonical distribution gives "nonequilibriumness"

$$D[\rho||\rho_{\mathrm{can}}(\alpha)] =< \log\frac{\rho}{\rho_{\mathrm{can}}(\alpha)}|\rho > \tag{2.10}$$

Now we derive work equality in information geometry. We rewrite Eq.(2.3) as follows,

$$\begin{aligned} W &= F_T(\alpha) - F_0(\alpha) - < F_T(\alpha) - H_T|\rho_T > + < F_0(\alpha) - H_0|\rho_0 > \\ &= \Delta F(\alpha) - \alpha^{-1} < \log \rho_{\mathrm{can},T}(\alpha)|\rho_T > + \alpha^{-1} < \log \rho_{\mathrm{can},0}(\alpha)|\rho_0 > \end{aligned} \tag{2.11}$$

where $\Delta F(\alpha) = F_T(\alpha) - F_0(\alpha)$. Using the conservation of the Gibb–Shanonn entropy,

$$\begin{aligned} W - \Delta F(\alpha) &= -\alpha^{-1} < \log \rho_{\mathrm{can},T}(\alpha)|\rho_T > - S_T \\ &+ \alpha^{-1} < \log \rho_{\mathrm{can},0}(\alpha)|\rho_0 > + S_0 \\ &= \alpha^{-1} D[\rho_T||\rho_{\mathrm{can},T}(\alpha)] - \alpha^{-1} D[\rho_0||\rho_{\mathrm{can},0}(\alpha)] \end{aligned} \tag{2.12}$$

We note that Eq.(2.12) is valid for any positive α.

2.3 The maximum work formulation in an adiabatic process

In this section we derive the maximum work formulation for an equilibrium initial state in an adiabatic process. By neglecting the reservoir we consider the system to be thermally isolated system, $H = H^{(\mathrm{S})}$ and $\rho = \rho^{(\mathrm{S})}$. The work equality Eq.(2.12) is rewritten as

$$W = \Delta F(\alpha) + \alpha^{-1} D[\rho_T || \rho_{\mathrm{can},T}(\alpha)] - \alpha^{-1} D[\rho_0 || \rho_{\mathrm{can},0}(\alpha)]. \tag{2.13}$$

It is clear that the work is uniquely determined since the both initial and final states are known.

For an unknown final state, the work equality can be rewritten as an inequality for a given initial state. The whole information regarding with the final state is included in the first relative entropy in Eq.(2.13). Therefore, we immediately obtain the following inequality using non-negativity of the relative entropy,

$$W \geq \Delta F(\alpha) - \alpha^{-1} D[\rho_0 || \rho_{\mathrm{can},0}(\alpha)]. \tag{2.14}$$

This inequality is valid for any final probability density, ρ_T.

This inequality is also valid for any positive α. Therefore, we define an effective temperature $\tilde{\beta}^{-1} = \alpha^{-1}$ for which the right-hand-side (RHS) of Eq.(2.14) is maximized. In order to maximize RHS, we first rewrite it as

$$\mathrm{RHS} = F_T(\alpha) - E_0 + \alpha^{-1} S_0. \tag{2.15}$$

After taking the derivative of RHS with respect to α^{-1} we obtain

$$\frac{d\mathrm{RHS}}{d\alpha^{-1}} = -S_{\mathrm{can},T}(\alpha) + S_0. \tag{2.16}$$

where we used

$$\frac{dF_T(\alpha)}{d\alpha^{-1}} = -S_{\mathrm{can},T}(\alpha). \tag{2.17}$$

From the monotonicity of the entropy of the canonical distribution, $S_{\mathrm{can},T}(\tilde{\alpha})$, the effective temperature is uniquely determined by the isentropic relation,

$$S_{\mathrm{can},T}(\tilde{\beta}) = S_0. \tag{2.18}$$

The uniqueness of the effective temperature is shown in Appendix C

We obtain the generalized maximum work formulation for a nonequilibrium initial state in an adiabatic process with the effective temperature,

$$W \geq \Delta F(\tilde{\beta}) - \tilde{\beta}^{-1} D[\rho_0 || \rho_{\mathrm{can},0}(\tilde{\beta})]. \tag{2.19}$$

We confirm that the generalized maximum work formulation returns to the maximum work formulation for an equilibrium initial state. Suppose the system is in equilibrium by connecting a reservoir with temperature β^{-1} in the past. We disconnect the system from the reservoir and make it thermally isolated. We start a periodic operation on it at $t = 0$. Then, the initial probability density is the canonical distribution with temperature β^{-1}. From the isentropic relation for a periodic operation,

$$S_{\mathrm{can},0}(\tilde{\beta}) = S_{\mathrm{can},T}(\tilde{\beta}) = S_0 = S_{\mathrm{can},0}(\beta), \tag{2.20}$$

the effective temperature $\tilde{\beta}^{-1}$ is the same as the temperature β^{-1}. Since the relative entropy vanishes, the original second law is reproduced

$$W \geq 0 \tag{2.21}$$

where we used $\Delta F(\beta) = 0$ for a periodic operation.

Let us discuss by what processes the maximum work is realized for a nonequilibrium initial state. To gain maximum work from a nonequilibrium initial state, we have to avoid dissipation. To prevent spontaneous relaxation, such as the free expansion of gas, the initial Hamiltonian should be instantaneously changed at the beginning of the process so that the initial state is a canonical distribution for the changed Hamiltonian. This canonical distribution can evolve to the final canonical distribution in a process that is dissipationless. The final Hamiltonian should be the initial Hamiltonian for a cyclic operation.

The generalized maximum work formulation is rewritten as

$$W \geq < H_T | \rho_{\mathrm{can},T}(\tilde{\beta}) > - < H_0 | \rho_0 > \tag{2.22}$$

where we substituted the isentropic relation into the relative entropy in Eq.(2.14).

We formally introduce a Hamiltonian, $\mathcal{H}_0$, for which the nonequilibrium initial probability density can be written as a canonical distribution, $\rho_0 = \exp[\tilde{\beta}\{\mathcal{F}_0(\tilde{\beta}) - \mathcal{H}_0\}]$ where $\mathcal{F}_0(\tilde{\beta})$ is the free energy for $\mathcal{H}_0$. Then, the maximum work, right-hand-side of Eq.(2.22) with the negative sign, is rewritten as

$$-W_{\max} = W_{\mathrm{IE}} + W_{\mathrm{IS}} \tag{2.23}$$

where

$$\begin{aligned} W_{\mathrm{IS}} &\equiv < \mathcal{H}_0 - H_0 | \rho_0 >, & (2.24) \\ W_{\mathrm{IE}} &\equiv < H_T | \rho_{\mathrm{can},T}(\tilde{\beta}) > - < \mathcal{H}_0 | \rho_0 > . & (2.25) \end{aligned}$$

The most efficient way to gain work from the nonequilibrium initial probability density in an adiabatic process is as follows:

(1) Change the initial Hamiltonian, H_0 to $\mathcal{H}_0$ for instantaneous stabilization (IS) of the initial probability density.

(2) Change $\mathcal{H}_0$ to the final Hamiltonian, H_T, in an isentropic process (IE).

Here we assume that the isentropic process exists.

2.4 The generalized maximum work formulation for a transition between nonequilibrium states in a process with a finite reservoir

In this section we consider a process in which the system is connected to the finite reservoir. We make the following two assumptions:
(1)The initial probability density is separable for the system and the reservoir as $\rho_0 = \rho_0^{(\mathrm{S})}\rho_0^{(\mathrm{R})}$.
(2)The final marginal probability density of the system is given but the final marginal probability density of the reservoir is unknown.

We start at Eq.(2.12). We rewrite the final relative entropy as follows,

$$D[\rho_T||\rho_{\mathrm{can},T}(\alpha)] = D[\rho_T||\rho_T^{(\mathrm{S})}\rho_T^{(\mathrm{R})}] + D[\rho_T^{(\mathrm{S})}||\rho_{\mathrm{can},T}^{(\mathrm{S})}(\alpha)] + D[\rho_T^{(\mathrm{R})}||\rho_{\mathrm{can}}^{(\mathrm{R})}(\alpha)]. \tag{2.26}$$

The derivation of Eq.(2.26) is shown in Appendix D. By substituting Eq.(2.26) into Eq.(2.12), the work equality is rewritten in terms of the final marginal probabilities,

$$\begin{aligned} W &= \Delta F(\alpha) + D[\rho_T||\rho_T^{(\mathrm{S})}\rho_T^{(\mathrm{R})}] + D[\rho_T^{(\mathrm{S})}||\rho_{\mathrm{can},T}^{(\mathrm{S})}(\alpha)] \\ &+ D[\rho_T^{(\mathrm{R})}||\rho_{\mathrm{can}}^{(\mathrm{R})}(\alpha)] - \alpha^{-1}D[\rho_0||\rho_{\mathrm{can},0}(\alpha)]. \end{aligned} \tag{2.27}$$

By neglecting the first and third relative entropies with respect to the final state of the reservoir, we obtain the following inequality,

$$W \geq \Delta F(\alpha) + \alpha^{-1}D[\rho_T^{(\mathrm{S})}||\rho_{\mathrm{can},T}^{(\mathrm{S})}(\alpha)] - \alpha^{-1}D[\rho_0||\rho_{\mathrm{can},0}(\alpha)]. \tag{2.28}$$

This inequality is valid for any positive α.

Similar to the argument in the previous section, we will determine the effective temperature for which the lower bound of the work is maximized. The right-hand-side(RHS) of Eq.(2.28) is rewritten to make clear the α dependence,

$$RHS = E_T^{(\mathrm{S})} - E_0 + F^{(\mathrm{R})}(\alpha) - \alpha^{-1}(S_T^{(\mathrm{S})} - S_0). \tag{2.29}$$

The derivative of RHS with respect to α^{-1} is,

$$\frac{d(\mathrm{RHS})}{d\alpha^{-1}} = -S_{\mathrm{can}}^{(\mathrm{R})}(\alpha) - S_T^{(\mathrm{S})} + S_0. \tag{2.30}$$

From the monotonicity of the entropy of the canonical distribution, the effective temperature is uniquely determined by the isentropic relation,

$$S_{\mathrm{can}}^{(\mathrm{R})}(\tilde{\beta}) + S_T^{(\mathrm{S})} = S_0. \tag{2.31}$$

With the effective temperature, the maximum work formulation is generalized for a transition between nonequilibrium states in a process with a finite reservoir,

$$W >\geq \Delta F(\tilde{\beta}) + \tilde{\beta}^{-1}D[\rho_T^{(\mathrm{S})}||\rho_{\mathrm{can},T}^{(\mathrm{S})}(\tilde{\beta})] - \tilde{\beta}^{-1}D[\rho_0||\rho_{\mathrm{can},0}(\tilde{\beta})]. \tag{2.32}$$

The dissipative work $W - \Delta F(\tilde{\beta})$ is bounded by the difference between the initial total relative entropy and the final relative entropy of the system. As discussed before, the relative entropy gives the “distance” from equilibrium. The dissipative work is bounded by the change of the “nonequilibriumness”.

Using the isentropic relation, Eq.(2.32) is also rewritten as,

$$W \geq E_T^{(\mathrm{S})} + < H^{(\mathrm{R})} | \rho_{\mathrm{can}}^{(\mathrm{R})}(\tilde{\beta}) > - E_0. \tag{2.33}$$

In the next section, we will use the equation to discuss by what processes the maximum work is realized in the next section.

2.5 The generalized maximum work formulation for a transition between nonequilibrium states in a quasi-isothermal process

The temperature is ordinarily defined for an infinite reservoir. We assume that the number of degrees of freedom of the reservoir, $N^{(\mathrm{R})}$, is much greater than the number of degrees of freedom of the system, $N^{(\mathrm{S})}$. In this section, we introduce an effective temperature, β^{-1}, of the reservoir realized after isentropic equilibration without contact with the system. Using this effective temperature we will rewrite the generalized maximum work formulation for a transition between nonequilibrium states in a process with a large but finite reservoir. We call this process a quasi-isothermal process.

From the following isentropic relation,

$$S^{(\mathrm{R})}_{\mathrm{can}}(\beta) \equiv S^{(\mathrm{R})}_0. \tag{2.34}$$

an effective temperature, β^{-1}, of the reservoir is determined. The effective temperature is realized after isentropic equilibration without contact with the system.

As assumed, the initial probability density of the total system is separable, $\rho_0 = \rho_0^{(\mathrm{S})}\rho_0^{(\mathrm{R})}$. Since the interaction Hamiltonian is negligible in the beginning,

$$E_0 = E_0^{(\mathrm{S})} + E_0^{(\mathrm{R})}. \tag{2.35}$$

Therfore, we rewrite Eq.(2.33) as

$$W \geq E_T^{(\mathrm{S})} - E_0^{(\mathrm{S})} + < H^{(\mathrm{R})} | \rho^{(R)}_{\mathrm{can}}(\tilde{\beta}) > - E_0^{(\mathrm{R})}. \tag{2.36}$$

Here,

$$\begin{aligned} < H^{(\mathrm{R})} | \rho^{(\mathrm{R})}_{\mathrm{can}}(\tilde{\beta}) > &= F^{(\mathrm{R})}(\tilde{\beta}) + \tilde{\beta}^{-1} S^{(\mathrm{R})}_{\mathrm{can}}(\tilde{\beta}) && (2.37)\\ &= F^{(\mathrm{R})}(\tilde{\beta}) + (\tilde{\beta}^{-1} - \beta^{-1}) S^{(\mathrm{R})}_{\mathrm{can}}(\tilde{\beta}) \\ &\qquad - \beta^{-1}\{S_T^{(\mathrm{S})} - S_0^{(\mathrm{S})}\} + \beta^{-1} S_0^{(\mathrm{R})}. && (2.38) \end{aligned}$$

where we used the isentropic relation, $S^{(\mathrm{R})}_{\mathrm{can}}(\tilde{\beta}) = -S_T^{(\mathrm{S})} + S_0^{(\mathrm{S})} + S_0^{(\mathrm{R})}$. Then, Eq.(2.36) is rewritten as,

$$W \geq E_T^{(\mathrm{S})} - E_0^{(\mathrm{S})} - \beta^{-1}\{S_T^{(\mathrm{S})} - S_0^{(\mathrm{S})}\} + \Delta W(\tilde{\beta}) + W^{(\mathrm{R})}_{\mathrm{EQ}} \tag{2.39}$$

where $\Delta W(\tilde{\beta})$ is a correction of the work for the finite reservoir,

$$\Delta W(\tilde{\beta}) \equiv F^{(\mathrm{R})}(\tilde{\beta}) - F^{(\mathrm{R})}(\beta) + (\tilde{\beta}^{-1} - \beta^{-1}) S^{(\mathrm{R})}_{\mathrm{can}}(\tilde{\beta}) \tag{2.40}$$

and $W^{(\mathrm{R})}_{\mathrm{EQ}}$ is the work for the isentropic equilibration without contact with the system,

$$W^{(\mathrm{R})}_{\mathrm{EQ}} \equiv < H^{(\mathrm{R})} | \rho^{(\mathrm{R})}_{\mathrm{can}}(\beta) > - E_0^{(\mathrm{R})}. \tag{2.41}$$

Because of energy conservation for the isentropic equilibration,

$$W^{(\mathrm{R})}_{\mathrm{EQ}} = 0. \tag{2.42}$$

The effective temperature must satisfy $< H^{(\mathrm{R})}|\rho^{(\mathrm{R})}_{\mathrm{can}}(\beta) >= E^{(\mathrm{R})}_0$.

We obtain the generalized maximum work formulation for a transition between nonequilibrium states in a quasi-isothermal process,

$$W \geq E^{(\mathrm{S})}_T - E^{(\mathrm{S})}_0 - \beta^{-1}\{S^{(\mathrm{S})}_T - S^{(\mathrm{S})}_0\} + \Delta W(\tilde{\beta}). \tag{2.43}$$

After the long but straightforward calculations mentioned in Appendix E, we obtain a simple expression of the correction of the work for the finite reservoir,

$$\Delta W(\tilde{\beta}) = \beta^{-1} D[\rho^{(\mathrm{R})}_{\mathrm{can}}(\tilde{\beta})||\rho^{(\mathrm{R})}_{\mathrm{can}}(\beta)] \geq 0. \tag{2.44}$$

Using the relation between the relative entropy and the Gibbs-Shannon entropy,

$$\beta^{-1} D[\rho_t||\rho^{(\mathrm{S})}_{\mathrm{can},t}(\beta)] = -\beta^{-1} S^{(\mathrm{S})}_t + E^{(\mathrm{S})}_t - F^{(\mathrm{S})}_t(\beta). \tag{2.45}$$

We finally obtain the generalized maximum work formulation for a transition between nonequilibrium state in a quasi-isothermal process in terms of the relative entropies,

$$\begin{aligned} W \quad &\geq \quad \Delta F^{(\mathrm{S})}(\beta) + \beta^{-1} D[\rho^{(\mathrm{S})}_T||\rho^{(\mathrm{S})}_{\mathrm{can},T}(\beta)] \\ &- \quad \beta^{-1} D[\rho^{(\mathrm{S})}_0||\rho^{(\mathrm{S})}_{\mathrm{can},0}(\beta)] + \Delta W(\tilde{\beta}). \end{aligned} \tag{2.46}$$

2.6 The generalized maximum work formulation for a transition between nonequilibrium states in an isothermal process

In this section, we generalize the maximum work formulation for a transition between nonequilibrium states in an isothermal process. The isothermal process is realized in the limit of the infinite reservoir.

We start at Eq.(2.46),

$$\begin{aligned} W &\geq \Delta F^{(\mathrm{S})}(\beta) + \beta^{-1} D[\rho_T^{(\mathrm{S})} || \rho_{\mathrm{can},T}^{(\mathrm{S})}(\beta)] \\ &- \beta^{-1} D[\rho_0^{(\mathrm{S})} || \rho_{\mathrm{can},0}^{(\mathrm{S})}(\beta)] + \Delta W(\tilde{\beta}). \end{aligned}$$

We choose the initial probability density of the reservoir as the canonical distribution with temperature, β^{-1}. The effective temperature is uniquely determined by the isentropic relation,

$$S_{\mathrm{can}}^{(\mathrm{R})}(\tilde{\beta}) + S_T^{(\mathrm{S})} = S_{\mathrm{can}}^{(\mathrm{R})}(\beta) + S_0^{(\mathrm{S})}. \tag{2.47}$$

From order estimations in regard to the degrees of freedom of both the system and reservoir,

$$\tilde{\beta} - \beta \sim O(N^{(\mathrm{S})}/N^{(\mathrm{R})}) \to 0 \tag{2.48}$$

in the limit of the infinite reservoir, $N^{(\mathrm{R})} \to \infty$.

The correction of the work for the finite reservoir is given in Eq.(2.40),

$$\Delta W(\tilde{\beta}) = F^{(\mathrm{R})}(\tilde{\beta}) - F^{(\mathrm{R})}(\beta) + (\tilde{\beta}^{-1} - \beta^{-1}) S_{\mathrm{can}}^{(\mathrm{R})}(\tilde{\beta}).$$

Using the relation, $S_{\mathrm{can}}^{(\mathrm{R})}(\beta) = -dF^{(\mathrm{R})}(\beta)/d\beta^{-1}$, it is easy to show that the terms of the first order, $O(\tilde{\beta}^{-1} - \beta^{-1})$, cancel in the Taylor expansion. In the limit of the infinite reservoir, the correction of the work vanishes,

$$\Delta W(\tilde{\beta}) \sim O(N^{(\mathrm{R})}(N^{(\mathrm{S})}/N^{(\mathrm{R})})^2) \to 0. \tag{2.49}$$

In the limit of the infinite reservoir, we obtain the generalized maximum work formulation for a transition between nonequilibrium states in an isothermal process as

$$W \geq \Delta F^{(\mathrm{S})}(\beta) + \beta^{-1} D[\rho_T^{(\mathrm{S})} || \rho_{\mathrm{can},T}^{(\mathrm{S})}(\beta)] - \beta^{-1} D[\rho_0^{(\mathrm{S})} || \rho_{\mathrm{can},0}^{(\mathrm{S})}(\beta)]. \tag{2.50}$$

We show by what processes the maximum work is realized in an isothermal process. We rewrite Eq.(2.50) as

$$W \geq E_T^{(\mathrm{S})} - E_0^{(\mathrm{S})} - \beta^{-1}\{S_T^{(\mathrm{S})} - S_0^{(\mathrm{S})}\}, \tag{2.51}$$

where we used the isentropic relation Eq.(2.47) to rewrite relative entropies in Eq.(2.50).

Similar to the previous argument, we formally introduce a Hamiltonian, $\mathcal{H}_0^{(\mathrm{S})}(\mathcal{H}_T^{(\mathrm{S})})$, for which the nonequlibrium initial (final) probability density can be written as a canonical distribution,

$\rho_0^{(\mathrm{S})}$ =exp$[\beta\{\mathcal{F}_0^{(\mathrm{S})}(\beta)-\mathcal{H}_0^{(\mathrm{S})}\}]$($\rho_T^{(\mathrm{S})}=\exp[\beta\{\mathcal{F}_T^{(\mathrm{S})}(\beta)-\mathcal{H}_T^{(\mathrm{S})}\}]$) where $\mathcal{F}_0^{(\mathrm{S})}(\beta)$ ($\mathcal{F}_T^{(\mathrm{S})}(\beta)$) is the free energy for $\mathcal{H}_0^{(\mathrm{S})}$ ($\mathcal{H}_T^{(\mathrm{S})}$). Then we obtain

$$-W_{\max}=W_{\mathrm{IR}}+W_{\mathrm{QI}}+W_{\mathrm{IS}} \tag{2.52}$$

where

$$\begin{aligned} W_{\mathrm{IS}} &\equiv <\mathcal{H}_0^{(\mathrm{S})}-H_0^{(\mathrm{S})}|\rho_0^{(\mathrm{S})}>, && (2.53)\\ W_{\mathrm{QI}} &\equiv \mathcal{F}_T^{(\mathrm{S})}(\beta)-\mathcal{F}_0^{(\mathrm{S})}(\beta), && (2.54)\\ W_{\mathrm{IR}} &\equiv <H_T^{(\mathrm{S})}-\mathcal{H}_T^{(\mathrm{S})}|\rho_T^{(\mathrm{S})}>. && (2.55)\end{aligned}$$

Interpreting each of these terms we see that the most efficient way to gain work from the nonequilibrium initial probability density in a process for two coupled Hamiltonian systems is as follows:
(1) Change the initial Hamiltonian, $H_0^{(\mathrm{S})}$, to $\mathcal{H}_0^{(\mathrm{S})}$ for instantaneous stabilization (IS) of the initial probability density.
(2) Change $\mathcal{H}_0^{(\mathrm{S})}$ to $\mathcal{H}_T^{(\mathrm{S})}$ in a quasi-static isothermal process (QI).
(3) Change $\mathcal{H}_T^{(\mathrm{S})}$ to the final Hamiltonian, $H_T^{(\mathrm{S})}$ for instantaneous release (IR) of the final probability density of the system.
Here we assumed that the quasi-static isothermal process exists.

2.7 The generalized Clausius relation for a transition between nonequilibrium states in an isothermal process

From the first law of thermodynamics, the absorbed heat is given as

$$Q \equiv E_T^{(\mathrm{S})} - E_0^{(\mathrm{S})} - W. \tag{2.56}$$

Using Eq.(2.43), the heat, Q, absorbed in a quasi-isothermal process is bounded from above,

$$Q \leq \beta^{-1}\{S_T^{(\mathrm{S})} - S_0^{(\mathrm{S})}\} - \Delta W(\tilde{\beta}). \tag{2.57}$$

Then, the maximum absorbed heat is obtained from the maximum work as

$$Q_{\mathrm{max}} = \beta^{-1}\{S_T^{(\mathrm{S})} - S_0^{(\mathrm{S})}\} - \Delta W(\tilde{\beta}). \tag{2.58}$$

Similarly, the heat, Q absorbed in an isothermal process is bounded from above,

$$Q \leq \beta^{-1}\{S_T^{(\mathrm{S})} - S_0^{(\mathrm{S})}\}. \tag{2.59}$$

The maximum absorbed heat is obtained as

$$Q_{\mathrm{max}} = \beta^{-1}\{S_T^{(\mathrm{S})} - S_0^{(\mathrm{S})}\}. \tag{2.60}$$

We generalise the Clausius relation for a transition between nonequilibrium states by using both the initial and final Gibbs-Shannon entropies instead of the entropies of the initial and final canonical distributions [8,14,37,38].

Chapter 3

N–level Quantum System

3.1 Generalized work relation for N–level quantum system

We consider a thermally isolated quantum Hamiltonian system. The Hamiltonian $H(\theta(t))$ depends on time t through the parameter $\theta(t)$ following a given protocol associated with an external operation to the system. Hereafter, we abbreviate $\theta_t = \theta(t)$ for convenience.

The time evolution of the system is governed by the quantum Liouville equation,

$$\mathrm{i}\hbar\frac{\partial\rho(t)}{\partial t} = [H(\theta_t), \rho(t)]. \tag{3.1}$$

The density matrix at time t is given as

$$\rho(t) = U(t)\rho(0)U(t)^{-1} \tag{3.2}$$

where the unitary time evolution operator $U(t) \equiv \mathrm{T}\exp(-\mathrm{i}\int_0^t H(\theta_{t'})dt'/\hbar)$ where T means the time ordered product.

The work on the thermally isolated system from $t = 0$ to $t = T$ is given as

$$W = \mathrm{Tr}[H(\theta_T)\rho(T)] - \mathrm{Tr}[H(\theta_0)\rho(0)]. \tag{3.3}$$

It is important to note that the maximum work done by the system corresponds to the lowest work done on the system in our definition. Hereafter we will discuss a lower bound of the work on the system.

In the generalized second law the canonical distribution plays a crucial role even outside the context of a system in contact with a heat reservoir. The canonical distribution expresses a connection between energy (the Hamiltonian) and information (the probability distribution). Its meaning is the equilibrium state in thermodynamics but it also has meaning in a thermally isolated system. We consider the canonical distribution with the inverse of temperature α, $\rho_{\mathrm{can}}(\alpha,\theta) = \exp[\alpha\{F(\alpha,\theta) - H(\theta)\}]$ where we choose the Boltzmann constant unity and $F(\alpha,\theta) \equiv -\alpha^{-1}\log(\mathrm{Tr}[\exp\{-\alpha H(\theta)\}])$ is the corresponding free energy. Our definition of the temperature includes the Boltzmann constant so that the dimension of our temperature is energy. Using the canonical distribution, we can rewrite the work as

$$W = \Delta F(\alpha) - \alpha^{-1}\mathrm{Tr}[\log(\rho_{\mathrm{can}}(\alpha,\theta_T))\rho(T)] + \alpha^{-1}\mathrm{Tr}[\log(\rho_{\mathrm{can}}(\alpha,\theta_0))\rho(0)] \quad (3.4)$$

where $\Delta F(\alpha) = F(\alpha,\theta_T) - F(\alpha,\theta_0)$.

The von Neumann entropy of the state at time t is defined as $S(t) \equiv -\mathrm{Tr}[\log(\rho(t))\rho(t)]$. Using the conservation of the von Neumann entropy under unitary time evolution, $S(T) = S(0)$, the work may be written as the important equality

$$W = \Delta F(\alpha) + \alpha^{-1}\mathrm{D}[\rho(T)||\rho_{\mathrm{can}}(\alpha,\theta_T)] - \alpha^{-1}\mathrm{D}[\rho(0)||\rho_{\mathrm{can}}(\alpha,\theta_0)] \quad (3.5)$$

where $\mathrm{D}[\rho||\sigma] \equiv \mathrm{Tr}[\{\log(\rho) - \log(\sigma)\}\rho]$ is the non-negative quantum relative entropy [12, 21]. This is an identity for any inverse of temperature α. In this equality the dissipative work $W - \Delta F(\alpha)$ is exactly given as the difference between the initial and the final "distance" from equilibrium with a temperature.

Using the non-negativity of the second term in the right-hand-side of Eq.(3.5), we obtain the generalized maximum work formulation for a nonequilibrium initial state,

$$W \geq \Delta F(\tilde{\beta}) - \tilde{\beta}^{-1}\mathrm{D}[\rho(0)||\rho_{\mathrm{can}}(\tilde{\beta},\theta_0)] \quad (3.6)$$

where the effective temperature $\tilde{\beta}^{-1}$ is uniquely determined by an isentropic condition: the von Neumann entropy for the final canonical distribution is equal to the initial von Neumann entropy $S_{\mathrm{can}}(\tilde{\beta},\theta_T) = S(0)$, which makes the right hand side of Eq.(3.6) maximum for $\alpha = \tilde{\beta}$.

From the isentropic condition, we can rewrite Eq.(3.6) as

$$W \geq \mathrm{Tr}[H(\theta_T)\rho_{\mathrm{can}}(\tilde{\beta},\theta_T)] - \mathrm{Tr}[\tilde{H}\rho(0)] + \mathrm{Tr}[(\tilde{H} - H(\theta_0))\rho(0)] \quad (3.7)$$

where an effective Hamiltonian $\tilde{H}$ is introduced to make the nonequilibrium initial state a canonical distribution: $\rho(0) = \exp[\tilde{\beta}\{\tilde{F}(\tilde{\beta}) - \tilde{H}\}]$ where $\tilde{F}(\tilde{\beta})$ is the corresponding free energy. The right hand side of the above inequality tells us how to realize the maximum work in two consecutive processes:

(1) An instantaneous stabilization process in which we instantaneously change the initial Hamiltonian to the effective Hamiltonian at the beginning to stop the time evolution from the nonequilibrium initial state;

(2) A restoration process in which the effective Hamiltonian is changed to the final one in an isentropic process.

3.2 Periodic operation to obtain the maximum work from the nonequilibrium initial state in a two–level quantum system I

Now we will focus on a two-level quantum system to obtain an efficient periodic operation that extracts the maximum work from a nonequilibrium initial state. We consider the following time-dependent Hamiltonian [34],

$$H(\theta) = \frac{\Delta\epsilon(\theta)}{2} \left(\begin{array}{cc} \cos(2\theta) & \sin(2\theta) \\ \sin(2\theta) & -\cos(2\theta) \end{array} \right). \tag{3.8}$$

The eigenvalues of the Hamiltonian are $\pm\Delta\epsilon(\theta)/2$. The probability amplitude for the ground state is $|0,\theta >= (-\sin(\theta), \cos(\theta))^{\mathrm{T}}$ and the probability amplitude for the excited state is $|1,\theta >= (\cos(\theta), \sin(\theta))^{\mathrm{T}}$. The superscript T means the transposition of the vector. We choose the zero energy as the middle of the two levels to make them symmetric.

We first consider time-independent energy levels, $\Delta\epsilon = \hbar\omega$ where ω is the constant angular frequency corresponding to the energy spacing. We choose the following parameter with linear time dependence for a given interval $t \in [a, b)$, $\theta_t = \Omega(t-a) + \theta_a$ where $\Omega = (\theta_b - \theta_a)/(b-a)$. For this linear time-dependent Hamiltonian one can exactly derive the transition probability, which is the Rabi formula [39].

We start with the following transition amplitudes,

$$\hat{a}_{k|j}(\theta_t) =< k, \theta_t|U_\theta(\theta_t)|j, \theta_a > \mathrm{e}^{\mathrm{i}(2k-1)\eta(\theta_t-\theta_a)} \quad j, k = 0, 1 \tag{3.9}$$

where $\eta \equiv \omega/(2\Omega)$ and $U_\theta(\theta_t) = \mathrm{T}\exp[-\mathrm{i}\int_{\theta_a}^{\theta_t} H(\theta)d\theta/(\hbar\Omega)]$. The time evolution operator $U_\theta(\theta_t)$ is the same as $U(t)$ previously defined. Since the transition amplitudes depend on time through the parameter, we introduced $U_\theta(\theta_t)$ to make the parameter dependence explicit. The phase factor was introduced to cancel out the parameter derivative of $U_\theta(\theta_t)$. Therefore, the θ_t dependence in the right-hand-side of Eq.(3.9) only appears in the bra-vector $< k, \theta_t|$. Now we take the derivative with respect to θ_t to both sides of Eq.(3.9).

$$\frac{d}{d\theta_t}\hat{a}_{k|j}(\theta_t) = \sum_{k'}\{\frac{d}{d\theta_t} < k, \theta_t|k', \theta' >\} < k', \theta'|U_\theta(\theta_t)|j, \theta_a > \mathrm{e}^{\mathrm{i}(2k-1)\eta(\theta_t-\theta_a)} \tag{3.10}$$

where we used the completeness relation $\sum_{k'} |k', \theta' >< k', \theta'| = 1$ for any θ'. Using the relation $\partial_\theta < k, \theta|j, \theta' >= (2k-1)\delta_{j,1-k}$ for $\theta' \to \theta$, we obtain the coupled differential equations with respect to θ,

$$\frac{d}{d\theta}\hat{a}_{k|j}(\theta) = (2k-1)\mathrm{e}^{\mathrm{i}2(2k-1)\eta(\theta-\theta_a)}\hat{a}_{1-k|j}(\theta). \tag{3.11}$$

The solutions for the initial conditions, $\hat{a}_{0|0}(\theta_a) = \hat{a}_{1|1}(\theta_a) = 1$, $\hat{a}_{0|1}(\theta_a) = \hat{a}_{1|0}(\theta_a) = 0$ are given as

$$\hat{a}_{0|1}(\theta) = -\hat{a}^*_{1|0}(\theta) = -\frac{\mathrm{e}^{-\mathrm{i}\eta(\theta-\theta_a)}}{\sqrt{1+\eta^2}}\sin((\theta-\theta_a)\sqrt{1+\eta^2}). \tag{3.12}$$

From Eq.(3.11), $\hat{a}_{0|0}(\theta)$ $(\hat{a}_{1|1}(\theta))$ is obtained from the derivatives of $\hat{a}_{1|0}(\theta)$ $(\hat{a}_{0|1}(\theta))$ with respect to θ.

The transition probability from the excited to the ground state is given as

$$P_{\mathrm{T}} = |\hat{a}_{0|1}(\theta_b)|^2 = 1 - |\hat{a}_{1|1}(\theta_b)|^2. \tag{3.13}$$

The survival probability is also given as $P_{\mathrm{S}} = 1 - P_{\mathrm{T}}$.

First we choose the pure excited state as a nonequilibrium initial state. This initial state is expected after energy measurement. The cyclic operation includes two processes:

(1) The stabilization process for $t \in [0, \tau)$ in which the pure excited state becomes the ground state, the canonical distribution with zero temperature, by changing $H(\theta_0 = 0)$ to $H(\theta_\tau = \pi/2) = -H(\theta_0 = 0)$;

(2) The restoration process to the original Hamiltonian without any transition to the excited state for $t \in [\tau, T)$. The final Hamiltonian is restored to the original Hamiltonian, $H(\theta_T) = H(\theta_0)$, for $\theta_T = \pi$ and $\theta_0 = 0$.

The transition probability for finite τ in the stabilization process is illustrated in Figure 3.1. When we take the limit of $\tau \to 0$, while keeping $\theta_0 = 0$ and $\theta_\tau = \pi/2$, the transition probability becomes 1 for $U(\theta_\tau, \tau) \to 1$ and the instantaneous stabilization is realized. In this limit the state does not change, $\rho(\tau) = \rho(0)$, but the energy switches sign, $H(\theta_\tau) = -H(\theta_0)$.

The survival probability in the restoration process is illustrated in Figure 3.2 where $T - \tau$ is the period of the restoration process. In the limit of the quasi-static process, $T - \tau \to \infty$, there is no transition to the excited state and the ground state is preserved. As is seen in Figure 3.2, there are shorter periods for a restoration that preserves the ground state ($P_{\mathrm{S}} = 1$). The shortest time for the restoration is realized by $\omega(T - \tau) = \sqrt{3}\pi$, where $\hat{a}^*_{1|0} = 0$ in Eq.(3.12) for $\theta - \theta_a = \pi/2$ and $\eta = \omega(T - \tau)/\pi$.

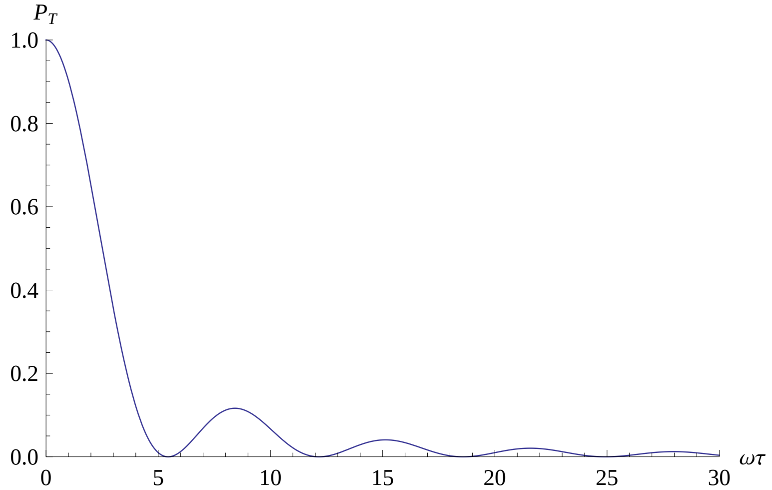

Figure 3.1: In the case of the constant energy levels, transition probability in the stabilization process for $\theta_0 = 0$ and $\theta_\tau = \pi/2$.

The previous argument can be generalized to an arbitrary nonequilibrium initial state. Without loss of generality, a nonequilibrium initial state can be

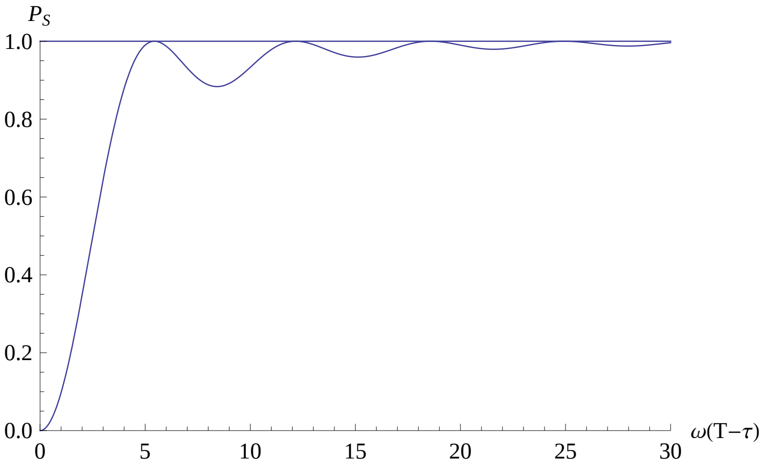

Figure 3.2: In the case of the constant energy levels, survival probability in the restoration process for $\theta_\tau = \pi/2$ and $\theta_T = \pi$.

written as the superposition of orthogonal pure states,

$$\begin{aligned} \rho(0) &= p_0|\psi_0 >< \psi_0| + p_1|\psi_1 >< \psi_1| \qquad (3.14) \\ |\psi_1 > &= |1,\theta_0 > \cos(\phi) + |0,\theta_0 > \sin(\phi) \\ |\psi_0 > &= -|1,\theta_0 > \sin(\phi) + |0,\theta_0 > \cos(\phi), \end{aligned}$$

where we define the zero-th and first pure states based on the occupation probability of the first pure state being equal or less than the zero-th, $p_0 \geq p_1 \geq 0$ $(p_0 + p_1 = 1)$. Since the states we consider are density matrices, they are operators in the Hilbert space of probability amplitudes; in particular, the pure state is a projection operator.

In the stabilization process, the dominant zero-th state is changed to the ground state. From the property of the unitary time evolution, the first state becomes the excited state after this stabilization process. Then, the state $\rho(\tau)$ becomes the canonical distribution with the effective temperature $\tilde{\beta}^{-1} = \hbar\omega/\log(p_0/p_1)$. To realize the instantaneous stabilization, we take the limit of $\tau \to 0$ while keeping $\theta_0 = 0$ and $\theta_\tau = \phi$. In this limit, $\rho(\tau) = \rho(0)$ and the Hamiltonian becomes the effective Hamiltonian given as

$$\tilde{H} = -\frac{\hbar\omega}{2}|\psi_0 >< \psi_0| + \frac{\hbar\omega}{2}|\psi_1 >< \psi_1|. \qquad (3.15)$$

The transition probability from the zero-th pure state to the ground state for finite τ, $P_{\mathrm{T}} = |-\hat{a}_{0|1}\sin(\phi) + \hat{a}_{0|0}\cos(\phi)|^2$, is illustrated in Figure 3.3.

In the restoration process, the final Hamiltonian is restored to the original Hamiltonian,
$H(\theta_T) = H(\theta_0)$, for $\theta_T = \pi$. As is seen in Figure 3.4, the shortest time to avoid any transition is realized by $\omega(T-\tau) = 2\sqrt{(2\pi-\phi)\phi}$ where $P_{\mathrm{S}} = |\hat{a}_{0|0}|^2 = 1$.

The maximum work is given as $W_{\max} = -\hbar\omega\sin^2(\phi)$. This is consistent with results in [32, 33]. At first glance we can extract the maximum energy

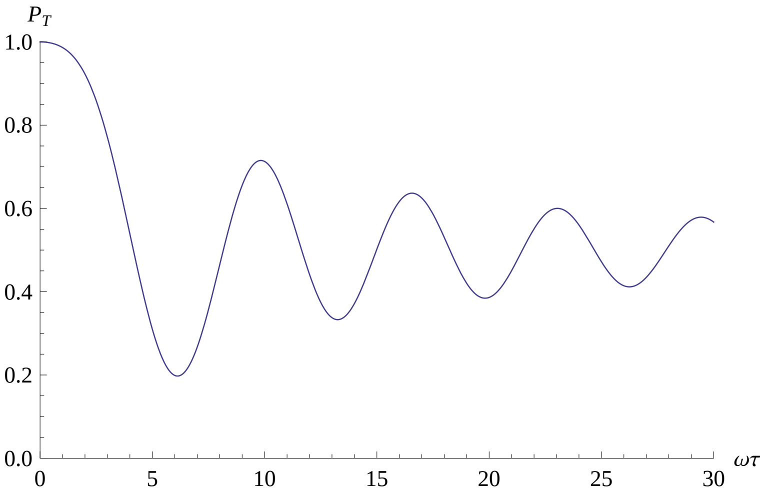

Figure 3.3: Transition probability in the stabilization process with the constant energy levels for $\theta_0 = 0$ and $\theta_\tau = \phi = 3\pi/4$.

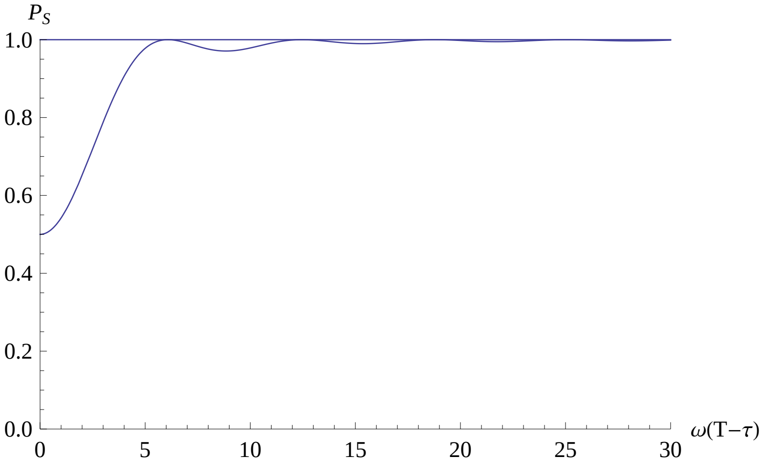

Figure 3.4: Survival probability in the restoration process with the constant energy levels for $\theta_\tau = 3\pi/4$ and $\theta_T = \pi$.

more efficiently for wider level spacing, $\hbar\omega$. However, it is important how long it takes to re-excite the state to extract the work repeatedly. The relaxation time is crucial for the re-excitation using a heat reservoir as will be discussed later.

3.3 Periodic operation to obtain the maximum work from the nonequilibrium initial state including an instantaneous stabilization II –the case of level crossing–

Now we consider an efficient periodic operation including a process with level crossing to obtain the maximum work. We choose $\Delta\epsilon = -2\hbar\omega\theta/\pi$ in the Hamiltonian. The eigenvalues of the Hamiltonian are $\pm\hbar\omega\theta/\pi$ so the level crossing occurs at $\theta = 0$. We choose the time-dependent parameter for $t \in [a, b)$ as $\theta_t = \Omega(t-a) + \theta_a$. As was shown by Allahverdyan and Nieuwenhuizen [34], the transition probability can be rigorously obtained even in a process with level crossing. Therefore we can explicitly show both the stabilization process and the restoration process.

We consider the following transition probability similar to the previous case,

$$\hat{a}_{k|j}(\theta_t) =< k, \theta_t|U(\theta_t, \Delta t)|j, \theta_a > \mathrm{e}^{-\mathrm{i}2(2k-1)\eta\int_{\theta_a}^{\theta_t}\theta_{t'}d\theta_{t'}/\pi} \quad j, k = 0, 1. \tag{3.16}$$

We obtain the coupled differential equations,

$$\frac{d}{d\theta}\hat{a}_{k|j}(\theta) = (2k-1)\mathrm{e}^{-\mathrm{i}2(2k-1)\eta(\theta^2-\theta_a^2)/\pi}\hat{a}_{1-k|j}(\theta). \tag{3.17}$$

The solutions can be written as

$$\hat{a}_{0|1}(\theta) = c_1\mathrm{He}(-\mathrm{i}\frac{\pi}{4\eta}, (-1)^{1/4}\theta\sqrt{\frac{2\eta}{\pi}}) + c_2\mathrm{F}_1(\mathrm{i}\frac{\pi}{8\eta}, \frac{1}{2}, \mathrm{i}\frac{2\theta^2\eta}{\pi}) \tag{3.18}$$

where c_1 and c_2 are constants, He is a Hermite polynomial, and F_1 is a confluent hypergeometric function of the first kind [40]. They are generalized for complex parameters and complex variable.

The transition probability from the initial excited state to the final ground state is given as $P_\mathrm{T} = |\hat{a}_{1|1}(\theta_b)|^2$ and the survival probability $P_\mathrm{S} = |\hat{a}_{0|1}(\theta_b)|^2 = 1 - P_\mathrm{T}$. Notice that the initial state is same as the final state in the transition probability. This comes from the fact that the initial excited state becomes the final ground state because of the level crossing.

We first consider the stabilization process for $t \in [0, \tau)$. The instantaneous stabilization can be realized even in a process with level crossing. For the nonequilibrium initial state defined in Eq.(3.15), we choose $\theta_0 = -\pi/2$ and $\theta_\tau = \phi > 0$ and take the limit of $\tau \to 0$. Then, $\rho(0) = \rho(\tau)$ and

$$H(\theta_\tau) = \tilde{H} = -\frac{\hbar\omega\theta_\tau}{\pi}|\psi_0 >< \psi_0| + \frac{\hbar\omega\theta_\tau}{\pi}|\psi_1 >< \psi_1|. \tag{3.19}$$

The transition probability for finite τ, $P_\mathrm{T} = |-\hat{a}_{1|1}\sin(\phi) + \hat{a}_{1|0}\cos(\phi)|^2$, is shown in Figure 3.5.

We consider the restoration process to the original Hamiltonian for $t \in [\tau, T)$. The restoration of the original Hamiltonian, $H(\theta_T) = H(\theta_0)$, is realized for $\theta_\tau = \phi$ and $\theta_T = -\pi/2$. We can make an efficient process without any transition between the two levels by choosing the interval $T - \tau$ for which $P_\mathrm{S} = |\hat{a}_{0|1}|^2 = 1$ as shown in Figure 3.6.

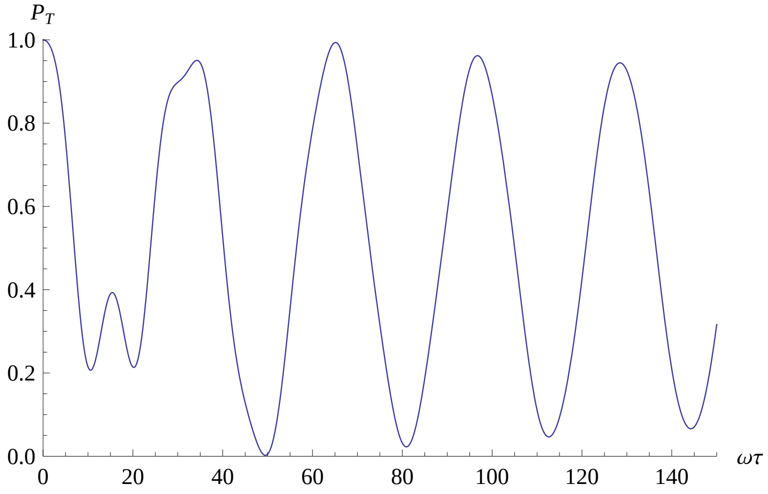

Figure 3.5: Transition probability in the stabilization process with level crossing for $\theta_0 = -\pi/2$ and $\theta_\tau = \phi = 3\pi/4$.

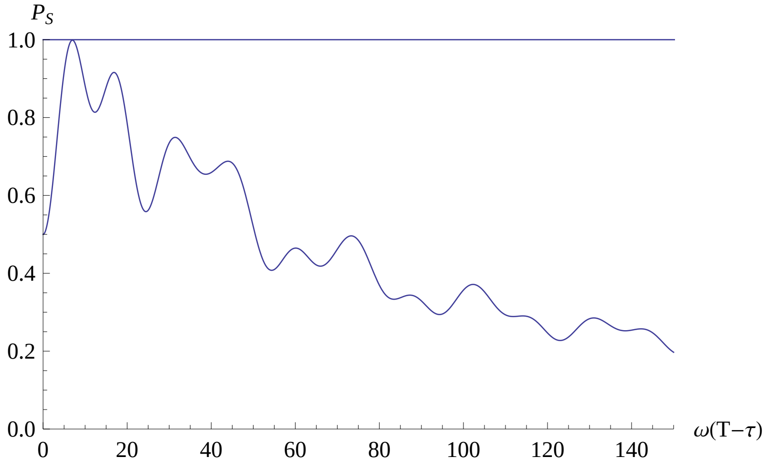

Figure 3.6: Survival probability in the restoration process with level crossing for $\theta_\tau = 3\pi/4$ and $\theta_T = -\pi/2$.

Using a non-quasi-static operation (As was pointed out by Allahverdyan and Nieuwenhuizen [34], if level crossing occurs work extraction is not always maximized by a quasi-static operation. such as the instantaneous stabilization we can extract the maximum work in a process with level crossing. The level crossing occurs within the stabilization process. Any effect of the level crossing turns out to be negligible in the instantaneous limit. The instantaneous stabilization was originally introduced to prevent spontaneous relaxation of a nonequilibrium thermodynamic system. It also prevents any loss of work in a process with level crossing for an N–level quantum system.)

3.4 Extension to an N–level system

In order to extend our argument for $N = 2$ to a general N we first have to modify the generalized maximum work formulation for a general N–level system. For $N = 2$, we can take any nonequilibrium initial state to the final canonical distribution by adjusting the effective temperature. However, we cannot do this for a greater N. The set of eigenvalues of the initial density matrix is preserved under a unitary time evolution. If we can take a nonequilibrium initial state to the final canonical distribution, the set of eigenvalues of the initial density matrix must be same as the set of the final canonical distribution in the diagonal representation. Since the final Hamiltonian (the set of final energy levels) is given, we cannot take an arbitrary nonequilibrium initial state to the final canonical distribution using any unitary time evolution.

Fortunately, we can take any nonequilibrium initial state to the final passive state and the second law for a passive initial state was established in an N–level quantum system [28, 29, 36, 31] A passive state satisfies the following properties: (1) It is simultaneously diagonalizable with the Hamiltonian so it can be written in terms of a sum of energy eigenstates; (2) It is determined by a series of occupation probabilities for each energy level. (Here we assume no degeneracy with respect to energy levels.); (3) The series of occupation probabilities is monotonically decreasing in the wide sense with respect to the level of energy. (The occupation probabilities of the nth energy level is equal or greater than the $n + 1$th energy level for $n = 0, 1, 2, ..., N - 1$.)

Similar to an initial canonical distribution, we can not obtain work from an initial passive state using any periodic operation,

$$\begin{aligned} W &= \mathrm{Tr}[H(\theta_T)\rho(T)] - \mathrm{Tr}[H(\theta_0)\rho_{\mathrm{passive}}(0)] \\ &\geq \mathrm{Tr}[H(\theta_T)\rho_{\mathrm{passive}}(T)] - \mathrm{Tr}[H(\theta_0)\rho_{\mathrm{passive}}(0)] \end{aligned} \tag{3.20}$$

where $\rho_{\mathrm{passive}}(t)$ is a passive state at time t.

Using the above inequality we obtain the generalized maximum work formulation for a nonequilibrium initial state in an N–level system as

$$\begin{aligned} W &= \mathrm{Tr}[H(\theta_T)\rho(T)] - \mathrm{Tr}[H(\theta_0)\rho(0)] \\ &\geq \mathrm{Tr}[H(\theta_T)\rho_{\mathrm{passive}}(T)] - \mathrm{Tr}[\tilde{H}\rho(0)] + \mathrm{Tr}[(\tilde{H} - H(\theta_0))\rho(0)] \end{aligned} \tag{3.21}$$

where $\tilde{H}$ is the effective Hamiltonian for which the nonequilibrium initial state is written as a passive state in terms of the effective Hamiltonian. The maximum work can be extracted in two consecutive processes: the instantaneous stabilization and an isentropic process such as a quantum quasi-static process from the effective passive state to the final passive state.

Finally, we consider a periodic operation to obtain the maximum work from a nonequilibrium initial state in an N–level system. The periodic operation is divided into two processes: the instantaneous stabilization and the restoration process to the original Hamiltonian.

Suppose both the initial Hamiltonian and the nonequilibrium initial distribution are written as a sum of pure eigenstates in each diagonal representation,

$$H(\theta_0) = \sum_{n=0}^{N-1} \epsilon_n |n, \theta_0 >< n, \theta_0| \tag{3.22}$$

$$\rho(0) = \sum_{j=0}^{N-1} p_j |\psi_j >< \psi_j| \tag{3.23}$$

where $\epsilon_n < \epsilon_{n+1}$ $(n = 0, 1, ..., N-1)$ and pure eigenstates, $|\psi_j >< \psi_j|$ $(j = 0, 1, ..., N-1)$, are ordered from the largest occupation probability p_0 to the smallest occupation probability p_{N-1}. Then, we choose the effective Hamiltonian as

$$\tilde{H} = \sum_{j=0}^{N-1} \epsilon_j |\psi_j >< \psi_j|. \tag{3.24}$$

The instantaneous stabilization is realized by instantaneously changing from the initial Hamiltonian to the effective Hamiltonian. The nonequilibrium initial state is kept in the sudden approximation as was explicitly shown for the two–level quantum system.

In the restoration process, we change the effective Hamiltonian to the original Hamiltonian.

The state remains passive without any transition during the minimum period $\hbar/\Delta\epsilon$ expected from the uncertainty relation.

3.5 An efficient quantum feedback control

To close this chapter, we comment on an efficient quantum feedback control using the instantaneous stabilizations. The system needs to be coupled to an energy source, such as a heat reservoir, to extract the maximum work repeatedly. We can obtain the maximum work from an initial excited state using the instantaneous stabilization. If the system is symmetric, such as a two–level quantum system, the Hamiltonian after the instantaneous stabilization is the same form as the original Hamiltonian. Then, we may skip the restoration process. After re-excitation by the energy source, we repeat the instantaneous stabilization. Since a real stabilization is an almost instantaneous process, we can control the system even though it is coupled to an energy source. The minimum period is determined by the re-excitation time, such as the relaxation time (Since our argument is not restricted within thermodynamics, we can choose any energy source such as light from sun to make the re-excitation time much shorter. We expect our efficient quantum process plays an important role in a quantum dot solar cell.)

We have to measure the quantum system to know if the system is in the excited state. The whole process including quantum measurements is called quantum feed back control [10, 27]. Toyabe *et al.* reported their experimental results [35]. We interpret their experiment as a demonstration of our efficient quantum feedback control using instantaneous stabilizations.

Chapter 4

Conclusions

In this thesis, we explicitly showed how to realize maximum work in a finite quantum system with the instantaneous stabilization. Instantaneous stabilization does not appear in traditional thermodynamics. We introduced instantaneous stabilization in order to extract the maximum work from the nonequilibrium initial state. The instantaneous stabilization prevented dissipation by spontaneous relaxation of the system. Since instantaneous stabilization was an ideal instantaneous process, its realizability was a crucial problem we needed to solve.

We considered a finite quantum system with a Hamiltonian that had a time dependence associated with an external cyclic operation. The first step in extracting work from the nonequilibrium initial state was to stop its time evolution. The initial Hamiltonian was changed to an effective Hamiltonian for which the nonequilibrium initial state was a stable canonical distribution. After the stabilization, we performed an isentropic process that changed the effective Hamiltonian to the final Hamiltonian. We showed in an exactly solvable two-level system how the maximum work was realized within the limit of instantaneous stabilization.

Our arguments were extended for a general N–level system. We confirmed that the generalized work relation is consistent with known results.

We showed how to extract the maximum work for a process that included a crossing of adiabatic energy levels. Work extracted from a thermally isolated equilibrium system was maximized for quasi-static realization of a given process. Allahverdyan and Nieuwenhuizen rigorously showed that this principle could be violated for a crossing of adiabatic energy levels. We gave a non-quasi-static process that maximized work extraction when there was a level crossing.

Finally we proposed an efficient quantum feedback control in a symmetric two–level quantum system connected to an energy source. We expected that our efficient quantum process plays an important role in the quantum dot solar cell.

Appendix A

Non-negativity of the relative entropy

The relative entropy is defined as

$$D[\rho_A||\rho_B] =< \log \frac{\rho_A}{\rho_B}|\rho_A > \tag{A.1}$$

where ρ_A and ρ_B are probability densities.

We assume the following inequality,

$$x - 1 \geq \log x. \tag{A.2}$$

Then,

$$\begin{aligned} -D[\rho_A||\rho_B] &= < \log \frac{\rho_B}{\rho_A}|\rho_A > \\ &\leq < \frac{\rho_B}{\rho_A} - 1|\rho_A > \\ &= < \rho_B - \rho_A > \\ &= 1 - 1 = 0 \end{aligned} \tag{A.3}$$

Appendix B

Non-negativity of the relative entropy in quantum mechanics

The relative entropy is defined in quantum mechanics as

$$D[\rho_A||\rho_B] = \mathrm{Tr}[(\log\rho_A - \log\rho_B)\rho_A] \tag{B.1}$$

where density matrices ρ_A and ρ_B are written as

$$\begin{aligned} \rho_A &= \sum_i |\varphi_i > \rho_{Ai} < \varphi_i|, && \text{(B.2)} \\ \rho_B &= \sum_i |\phi_i > \rho_{Bi} < \phi_i|. && \text{(B.3)} \end{aligned}$$

From the normalization of density matrices,

$$\begin{aligned} 1 &= \mathrm{Tr}[\rho_B] \\ &= \mathrm{Tr}[\rho_B \rho_A^{-1} \rho_A] \\ &= \sum_{i,j} < \varphi_i|\phi_j > \rho_{Bj} < \phi_j|\varphi_i > \rho_{Ai}^{-1}\rho_{Ai} \\ &= \sum_{i,j} \rho_{Bj}\rho_{Ai}^{-1}| < \phi_j|\varphi_i > |^2 \rho_{Ai}. && \text{(B.4)} \end{aligned}$$

We define $P_{j,i} = | < \phi_j|\varphi_i > |^2\rho_{Ai}$.

$$\begin{aligned} P_{j,i} &> 0, && \text{(B.5)} \\ \sum_{j,i} P_{j,i} &= \sum_{i,j} < \varphi_i|\phi_j >< \phi_j|\varphi_i > \rho_{Ai} \\ &= \sum_i < \varphi_i|\varphi_i > \rho_{Ai} \\ &= \sum_i \rho_{Ai} = 1. && \text{(B.6)} \end{aligned}$$

Then,

$$\begin{aligned}1 &= \sum_{i,j} \rho_{Bj}\rho_{Ai}^{-1} P_{i,j} \\ &= \sum_{i,j} \exp[-\log(\rho_{Bj}\rho_{Ai}^{-1})] P_{i,j} \\ &\geq \exp[-\sum_{i,j} \log(\rho_{Bj}\rho_{Ai}^{-1}) P_{i,j}] \end{aligned} \tag{B.7}$$

where we used the Jensen inequality, $< \mathrm{e}^x > \geq \mathrm{e}^{<x>}$. By taking logarithm on both sides,

$$\begin{aligned}0 &\leq \sum_{i,j} \log(\rho_{Bj}\rho_{Ai}^{-1}) P_{i,j} \\ &= \sum_{i,j} (\log \rho_{Bj} - \log \rho_{Ai}) | < \phi_j | \varphi_i > |^2 \rho_{Ai} \\ &= \mathrm{Tr}[(\log \rho_A - \log \rho_B)\rho_A]. \end{aligned} \tag{B.8}$$

Finally we obtain,

$$D[\rho_A || \rho_B] = \mathrm{Tr}[(\log \rho_A - \log \rho_B)\rho_A] \geq 0. \tag{B.9}$$

Appendix C

Uniqueness of the effective temperature

In this appendix, we show that the isentropic relation Eq.(2.18) uniquely determines the effective temperature. We start at Eq.(C.1),

$$\mathrm{RHS} = F_T(\alpha) - E_0 + \alpha^{-1} S_0.$$

The derivative of RHS with respect to α^{-1} is

$$\begin{aligned}\frac{d\mathrm{RHS}}{d\alpha^{-1}} &= \frac{dF_T(\alpha)}{d\alpha^{-1}} + S_0 \\ &= -S_{\mathrm{can},T}(\alpha) + S_0 \end{aligned} \tag{C.1}$$

where we used

$$\begin{aligned}\frac{dF(\alpha)}{d\alpha^{-1}} &= -\alpha^2 \frac{dF(\alpha)}{d\alpha} \\ &= -\alpha^2 \frac{d}{d\alpha}(-\frac{1}{\alpha} \log \int_\Gamma \exp(-\alpha H) dx) \\ &= \alpha F(\alpha) - \alpha < H|\rho_{\mathrm{can}}(\alpha) > \\ &= -S_{\mathrm{can}}(\alpha)\end{aligned} \tag{C.2}$$

The effective temperature is uniquely determined by the following two properties.
(1) Monotonicity of the entropy of the canonical distribution

$$\begin{aligned}\frac{dS_{\mathrm{can}}(\alpha)}{d\alpha} &= -\frac{d}{d\alpha}\alpha(F(\alpha) - < H|\rho_{\mathrm{can}}(\alpha) >) \\ &= -\alpha^{-1} S_{\mathrm{can}}(\alpha) - \alpha \frac{dF(\alpha)}{\alpha} + \alpha \frac{d < H|\rho_{\mathrm{can}}(\alpha) >}{d\alpha} \\ &= -\alpha < \Delta H^2 |\rho_{\mathrm{can}}(\alpha) > \leq 0\end{aligned} \tag{C.3}$$

where

$$< \Delta H^2 |\rho_{\mathrm{can}}(\alpha) > = < (H - E_{\mathrm{can}}(\alpha))^2 |\rho_{\mathrm{can}}(\alpha) >, \tag{C.4}$$

$$E_{\mathrm{can}}(\alpha) = < H|\rho_{\mathrm{can}}(\alpha) > \tag{C.5}$$

(2) $S_{\mathrm{can},T}(0) \geq S_0 \geq S_{\mathrm{can},T}(\infty)$
For $\alpha \to 0$, $S_{\mathrm{can},T}(\alpha)$ becomes the maximum entropy of the uniform probability density so that $S_{\mathrm{can},T}(0) \geq S_T = S_0$ where we used the conservation of the entropy. For $\alpha \to \infty$, $S_{\mathrm{can},T}(\alpha)$ becomes the minimum entropy of the ground state so that $S_T = S_0 \geq S_{\mathrm{can},T}(\infty)$.

Appendix D

Derivation of Eq.(2.26)

$$
\begin{aligned}
D[\rho_T||\rho_T^{(\mathrm{S})}\rho_T^{(\mathrm{R})}] &=< \log(\frac{\rho_T}{\rho_T^{(\mathrm{S})}\rho_T^{(\mathrm{R})}})|\rho_T > \\
&=< \log\rho_T|\rho_T > - < \log\rho_T^{(\mathrm{S})}|\rho_T > - < \log\rho_T^{(\mathrm{R})}|\rho_T > \\
&=< \log\rho_T|\rho_T > - < \log\rho_T^{(\mathrm{S})}|\rho_T^{(\mathrm{S})} > - < \log\rho_T^{(\mathrm{R})}|\rho_T^{(\mathrm{R})} > \\
&=< \log\rho_T|\rho_T > - < \log\rho_{\mathrm{can},T}(\alpha)|\rho_T > + < \log\rho_{\mathrm{can},T}(\alpha)|\rho_T > \\
&\qquad - < \log\rho_T^{(\mathrm{S})}|\rho_T^{(\mathrm{S})} > - < \log\rho_T^{(\mathrm{R})}|\rho_T^{(\mathrm{R})} > \\
&= D[\rho_T||\rho_{\mathrm{can},T}(\alpha)] + < \log(\rho_{\mathrm{can},T}^{(\mathrm{S})}(\alpha)\rho_{\mathrm{can},T}^{(\mathrm{R})}(\alpha))|\rho_T > \\
&\qquad - < \log\rho_T^{(\mathrm{S})}|\rho_T^{(\mathrm{S})} > - < \log\rho_T^{(\mathrm{R})}|\rho_T^{(\mathrm{R})} > \\
&= D[\rho_T||\rho_{\mathrm{can},T}(\alpha)] + < \log\rho_{\mathrm{can},T}^{(\mathrm{S})}(\alpha)|\rho_T > - < \log\rho_T^{(\mathrm{S})}|\rho_T^{(\mathrm{S})} > \\
&\qquad + < \log\rho_{\mathrm{can},T}^{(\mathrm{R})}(\alpha)|\rho_T > - < \log\rho_T^{(\mathrm{R})}|\rho_T^{(\mathrm{R})} > \\
&= D[\rho_T||\rho_{\mathrm{can},T}(\alpha)] + < \log\rho_{\mathrm{can},T}^{(\mathrm{S})}(\alpha)|\rho_T^{(\mathrm{S})} > - < \log\rho_T^{(\mathrm{S})}|\rho_T^{(\mathrm{S})} > \\
&\qquad + < \log\rho_{\mathrm{can},T}^{(\mathrm{R})}(\alpha)|\rho_T^{(\mathrm{R})} > - < \log\rho_T^{(\mathrm{R})}|\rho_T^{(\mathrm{R})} > \\
&= D[\rho_T||\rho_{\mathrm{can},T}(\alpha)] - D[\rho_T^{(\mathrm{S})}||\rho_{\mathrm{can},T}^{(\mathrm{S})}(\alpha)] - D[\rho_T^{(\mathrm{R})}||\rho_{\mathrm{can},T}^{(\mathrm{R})}(\alpha)]
\end{aligned}
\tag{D.1}
$$

Appendix E

Derivation of Eq.(2.44)

$$\begin{aligned}
\Delta W(\tilde{\beta}) &= F_T^{(\mathrm{R})}(\tilde{\beta}) - F_T^{(\mathrm{R})}(\beta) + (\beta^{-1} - \tilde{\beta}^{-1}) < \log \rho_{\mathrm{can},T}^{(\mathrm{R})}(\tilde{\beta}) | \rho_{\mathrm{can},T}^{(\mathrm{R})}(\tilde{\beta}) > \\
&= F_T^{(\mathrm{R})}(\tilde{\beta}) - F_T^{(\mathrm{R})}(\beta) - \tilde{\beta}^{-1} < \log \rho_{\mathrm{can},T}^{(\mathrm{R})}(\tilde{\beta}) | \rho_{\mathrm{can},T}^{(\mathrm{R})}(\tilde{\beta}) > \\
&\qquad\qquad\qquad + \beta^{-1} < \log \rho_{\mathrm{can},T}^{(\mathrm{R})}(\tilde{\beta}) | \rho_{\mathrm{can},T}^{(\mathrm{R})}(\tilde{\beta}) > \\
&= F_T^{(\mathrm{R})}(\tilde{\beta}) - F_T^{(\mathrm{R})}(\beta) - F_T^{(\mathrm{R})}(\tilde{\beta}) + < H_T^{(\mathrm{R})} | \rho_{\mathrm{can},T}^{(\mathrm{R})}(\tilde{\beta}) > \\
&\qquad\qquad\qquad + \beta^{-1} < \log \rho_{\mathrm{can},T}^{(\mathrm{R})}(\tilde{\beta}) | \rho_{\mathrm{can},T}^{(\mathrm{R})}(\tilde{\beta}) > \\
&= -F_T^{(\mathrm{R})}(\beta) + < H_T^{(\mathrm{R})} | \rho_{\mathrm{can},T}^{(\mathrm{R})}(\tilde{\beta}) > + \beta^{-1} < \log \rho_{\mathrm{can},T}^{(\mathrm{R})}(\tilde{\beta}) | \rho_{\mathrm{can},T}^{(\mathrm{R})}(\tilde{\beta}) > \\
&= -\beta^{-1} < \beta F_T^{(\mathrm{R})}(\beta) - \beta H_T^{(\mathrm{R})} | \rho_{\mathrm{can},T}^{(\mathrm{R})}(\tilde{\beta}) > \\
&\qquad\qquad\qquad + \beta^{-1} < \log \rho_{\mathrm{can},T}^{(\mathrm{R})}(\tilde{\beta}) | \rho_{\mathrm{can},T}^{(\mathrm{R})}(\tilde{\beta}) > \\
&= -\beta^{-1} < \log \rho_{\mathrm{can},T}^{(\mathrm{R})}(\beta) | \rho_{\mathrm{can},T}^{(\mathrm{R})}(\tilde{\beta}) > + \beta^{-1} < \log \rho_{\mathrm{can},T}^{(\mathrm{R})}(\tilde{\beta}) | \rho_{\mathrm{can},T}^{(\mathrm{R})}(\tilde{\beta}) > \\
&= \beta^{-1} < \log\left(\frac{\rho_{\mathrm{can},T}^{(\mathrm{R})}(\tilde{\beta})}{\rho_{\mathrm{can},T}^{(\mathrm{R})}(\beta)}\right) | \rho_{\mathrm{can},T}^{(\mathrm{R})}(\tilde{\beta}) > \\
&= \beta^{-1} D[\rho_{\mathrm{can},T}^{(\mathrm{R})}(\tilde{\beta}) || \rho_{\mathrm{can},T}^{(\mathrm{R})}(\beta)] \geq 0. \qquad \text{(E.1)}
\end{aligned}$$

Appendix F

Derivations of Eq.(3.11) and Eq.(3.12)

We start at Eq.(3.9),

$$\hat{a}_{k|j}(\theta_t) =< k, \theta_t|U_\theta(\theta_t)|j, \theta_a > \mathrm{e}^{\mathrm{i}(2k-1)\eta(\theta_t-\theta_a)} \quad j, k = 0, 1$$

where $\theta_t - \theta_a = \Omega(t-a)$, $\eta = \omega/(2\Omega)$ and

$$U_\theta(\theta_t) = \mathrm{T}\exp[-\mathrm{i}\int_{\theta_a}^{\theta_t} H(\theta)d\theta/(\hbar\Omega)].$$

We choose the phase factor to satisfy

$$< k, \theta_t|\frac{d}{d\theta_t}\{U_\theta(\theta_t)|j, \theta_a > \mathrm{e}^{\mathrm{i}(2k-1)\eta(\theta_t-\theta_a)}\} = 0 \tag{F.1}$$

where

$$\begin{aligned}
&< k, \theta_t|\frac{dU_\theta(\theta_t)}{d\theta_t}|j, \theta_a > \mathrm{e}^{\mathrm{i}(2k-1)\eta(\theta_t-\theta_a)} \\
&= - < k, \theta_t|\frac{\mathrm{i}H(\theta_t)}{\hbar\Omega}U_\theta(\theta_t)|j, \theta_a > \mathrm{e}^{\mathrm{i}(2k-1)\eta(\theta_t-\theta_a)} \\
&= - < k, \theta_t|\frac{\mathrm{i}(2k-1)\omega}{2\Omega}U_\theta(\theta_t)|j, \theta_a > \mathrm{e}^{\mathrm{i}(2k-1)\eta(\theta_t-\theta_a)} \\
&= - < k, \theta_t|U_\theta(\theta_t)|j, \theta_a > \mathrm{i}(2k-1)\eta\mathrm{e}^{\mathrm{i}(2k-1)\eta(\theta_t-\theta_a)} \\
&= - < k, \theta_t|U_\theta(\theta_t)|j, \theta_a > \frac{d}{d\theta_t}\mathrm{e}^{\mathrm{i}(2k-1)\eta(\theta_t-\theta_a)}
\end{aligned} \tag{F.2}$$

where we used $H(\theta_t)|k, \theta_t >= (2k-1)\hbar\omega/2|k, \theta_t >$. Therefore,

$$\begin{aligned}
\frac{d}{d\theta_t}\hat{a}_{k|j}(\theta_t) &= \{\frac{d}{d\theta_t} < k, \theta_t|\}U_\theta(\theta_t)|j, \theta_a > \mathrm{e}^{\mathrm{i}(2k-1)\eta(\theta_t-\theta_a)} \\
&= \sum_{m=0}^{1}\{\frac{d}{d\theta_t} < k, \theta_t|\}|m, \theta_t >< m, \theta_t|U_\theta(\theta_t)|j, \theta_a > \mathrm{e}^{\mathrm{i}(2k-1)\eta(\theta_t-\theta_a)} \\
&= -\sum_{m=0}^{1}\{< k, \theta_t|\frac{d}{d\theta_t}|m, \theta_t >\} < m, \theta_t|U_\theta(\theta_t)|j, \theta_a > \mathrm{e}^{\mathrm{i}(2k-1)\eta(\theta_t-\theta_a)}.
\end{aligned} \tag{F.3}$$

Using the relation, $< k,\theta_t|\frac{d}{d\theta_t}|m,\theta_t >= -(2k-1)\delta_{m,1-k}$, we obtain Eq.(3.11),

$$\begin{aligned}\frac{d}{d\theta_t}\hat{a}_{k|j}(\theta_t) &= (2k-1) < 1-k,\theta_t|U_\theta(\theta_t)|j,\theta_a > \mathrm{e}^{\mathrm{i}(2k-1)\eta(\theta_t-\theta_a)}\\ &= (2k-1)\mathrm{e}^{\mathrm{i}2(2k-1)\eta(\theta_t-\theta_a)}a_{1-k|j}(\theta_t).\end{aligned}$$

For $j=0$ and $k=1,0$,

$$\frac{d}{d\theta_t}\hat{a}_{1|0}(\theta_t) = \mathrm{e}^{\mathrm{i}2\eta(\theta_t-\theta_a)}\hat{a}_{0|0}(\theta_t), \tag{F.4}$$

$$\frac{d}{d\theta_t}\hat{a}_{0|0}(\theta_t) = -\mathrm{e}^{-\mathrm{i}2\eta(\theta_t-\theta_a)}\hat{a}_{1|0}(\theta_t). \tag{F.5}$$

Using these equations,

$$\begin{aligned}\frac{d^2}{d\theta_t^2}\hat{a}_{1|0}(\theta_t) &= \frac{d}{d\theta_t}\mathrm{e}^{\mathrm{i}2\eta(\theta_t-\theta_a)}\hat{a}_{0|0}(\theta_t)\\ &= \{\frac{d}{d\theta_t}\mathrm{e}^{\mathrm{i}2\eta(\theta_t-\theta_a)}\}\hat{a}_{0|0}(\theta_t) + \mathrm{e}^{\mathrm{i}2\eta(\theta_t-\theta_a)}\frac{d}{d\theta_t}\hat{a}_{0|0}(\theta_t)]\\ &= 2\mathrm{i}\eta\mathrm{e}^{\mathrm{i}2\eta(\theta_t-\theta_a)}\hat{a}_{0|0}(\theta_t) - \hat{a}_{1|0}(\theta_t)\\ &= 2\mathrm{i}\eta\frac{d}{d\theta_t}\hat{a}_{1|0}(\theta_t) - \hat{a}_{1|0}(\theta_t).\end{aligned} \tag{F.6}$$

$\hat{a}_{1|0}(\theta_t)$ satisfies the following differential equation,

$$\frac{d^2}{d\theta_t^2}\hat{a}_{1|0}(\theta_t) - 2\mathrm{i}\eta\frac{d}{d\theta_t}\hat{a}_{1|0}(\theta_t) + \hat{a}_{1|0}(\theta_t) = 0. \tag{F.7}$$

A general solutions is written as

$$\hat{a}_{1|0}(\theta_t) = c_1\mathrm{e}^{\mathrm{i}(\eta-\sqrt{1+\eta^2})\theta_t} + c_2\mathrm{e}^{\mathrm{i}(\eta+\sqrt{1+\eta^2})\theta_t}. \tag{F.8}$$

where c_1 and c_2 are constants. For the initial condition,

$$\hat{a}_{1|0}(\theta_a) = c_1\mathrm{e}^{\mathrm{i}(\eta-\sqrt{1+\eta^2})\theta_a} + c_2\mathrm{e}^{\mathrm{i}(\eta+\sqrt{1+\eta^2})\theta_a} = 0, \tag{F.9}$$

the coefficients c_1 and c_2 are rewritten as

$$c_1 = c\mathrm{e}^{-\mathrm{i}(\eta-\sqrt{1+\eta^2})\theta_a}, \tag{F.10}$$

$$c_2 = -c\mathrm{e}^{-\mathrm{i}(\eta+\sqrt{1+\eta^2})\theta_a}. \tag{F.11}$$

By substituting these results to Eq.(F.8),

$$\hat{a}_{1|0}(\theta_t) = c(\mathrm{e}^{\mathrm{i}(\eta-\sqrt{1+\eta^2})(\theta_t-\theta_a)} - \mathrm{e}^{\mathrm{i}(\eta+\sqrt{1+\eta^2})(\theta_t-\theta_a)}). \tag{F.12}$$

For the initial condition, $\hat{a}_{0|0}(\theta_a) = 0$,

$$\begin{aligned}\hat{a}_{0|0}(\theta_a) &= \frac{d}{d\theta_t}\hat{a}_{1|0}(\theta_t)|_{\theta_t=\theta_a}\\ &= \frac{d}{d\theta_t}c(\mathrm{e}^{\mathrm{i}(\eta-\sqrt{1+\eta^2})(\theta_t-\theta_a)} - \mathrm{e}^{\mathrm{i}(\eta+\sqrt{1+\eta^2})(\theta_t-\theta_a)})|_{\theta_t=\theta_a}\\ &= -2\mathrm{i}c\sqrt{1+\eta^2} = 1.\end{aligned}$$

The coefficient is determined as $c = -\frac{1}{2\mathrm{i}\sqrt{1+\eta^2}}$. By substituting this to Eq.(F.12),

$$\hat{a}_{1|0}(\theta_t) = \frac{\mathrm{e}^{\mathrm{i}\eta(\theta-\theta_0)}}{\sqrt{1+\eta^2}} \sin[\sqrt{1+\eta^2}(\theta-\theta_0)]. \tag{F.13}$$

For the initial conditions, $\hat{a}_{0|0}(\theta_a) = \hat{a}_{1|1}(\theta_a) = 1$ and $\hat{a}_{0|1}(\theta_a) = \hat{a}_{1|0}(\theta_a) = 0$, we finally obtain Eq.(3.12)

$$\hat{a}_{0|1}(\theta) = -\hat{a}^*_{1|0}(\theta) = -\frac{\mathrm{e}^{-\mathrm{i}\eta(\theta-\theta_a)}}{\sqrt{1+\eta^2}} \sin((\theta-\theta_a)\sqrt{1+\eta^2}). \tag{F.14}$$

From Eq.(3.11), $\hat{a}_{0|0}(\theta)$ ($\hat{a}_{1|1}(\theta)$) is obtained from the derivatives of $\hat{a}_{1|0}(\theta)$ ($\hat{a}_{0|1}(\theta)$) with respect to θ.

Appendix G

Derivations of Eq.(3.17) and Eq.(3.18)

We start at Eq.(3.16),

$$\hat{a}_{k|j}(\theta_t) =< k,\theta_t|U(\theta_t,\Delta t)|j,\theta_a > \mathrm{e}^{-\mathrm{i}2(2k-1)\eta\int_{\theta_a}^{\theta_t}\theta_{t'}d\theta_{t'}/\pi} \quad j,k=0,1.$$

where $\theta_t-\theta_a=\Omega(t-a)$, $\eta=\omega/(2\Omega)$ and

$$U_\theta(\theta_t)=\mathrm{T}\exp[-\mathrm{i}\int_{\theta_a}^{\theta_t}H(\theta)d\theta/(\hbar\Omega)].$$

We choose the phase factor to satisfy

$$< k,\theta_t|\frac{d}{d\theta_t}\{U_\theta(\theta_t)|j,\theta_a > \mathrm{e}^{-\mathrm{i}2(2k-1)\eta\int_{\theta_a}^{\theta_t}\theta_{t'}d\theta_{t'}/\pi}\}=0 \tag{G.1}$$

where

$$\begin{aligned}
&< k,\theta_t|\frac{dU_\theta(\theta_t)}{d\theta_t}|j,\theta_a > \mathrm{e}^{-\mathrm{i}2(2k-1)\eta\int_{\theta_a}^{\theta_t}\theta_{t'}d\theta_{t'}/\pi}\\
&=-< k,\theta_t|\frac{\mathrm{i}H(\theta_t)}{\hbar\Omega}U_\theta(\theta_t)|j,\theta_a > \mathrm{e}^{-\mathrm{i}2(2k-1)\eta\int_{\theta_a}^{\theta_t}\theta_{t'}d\theta_{t'}/\pi}\\
&=< k,\theta_t|\frac{\mathrm{i}(2k-1)\omega\theta_t}{\pi\Omega}U_\theta(\theta_t)|j,\theta_a > \mathrm{e}^{-\mathrm{i}2(2k-1)\eta\int_{\theta_a}^{\theta_t}\theta_{t'}d\theta_{t'}/\pi}\\
&=< k,\theta_t|U_\theta(\theta_t)|j,\theta_a > \mathrm{i}2(2k-1)\eta\theta_t/\pi\mathrm{e}^{-\mathrm{i}2(2k-1)\eta\int_{\theta_a}^{\theta_t}\theta_{t'}d\theta_{t'}/\pi}\\
&=-< k,\theta_t|U_\theta(\theta_t)|j,\theta_a > \frac{d}{d\theta_t}\mathrm{e}^{-\mathrm{i}2(2k-1)\eta\int_{\theta_a}^{\theta_t}\theta_{t'}d\theta_{t'}/\pi}
\end{aligned} \tag{G.2}$$

where we used $H(\theta_t)|k,\theta_t >= -(2k-1)\hbar\omega\theta/\pi|k,\theta_t >$. Therefore,

$$\begin{aligned}
&\frac{d}{d\theta_t}\hat{a}_{k|j}(\theta_t) = \{\frac{d}{d\theta_t} < k,\theta_t|\}U_\theta(\theta_t)|j,\theta_a > \mathrm{e}^{-\mathrm{i}2(2k-1)\eta\int_{\theta_a}^{\theta_t}\theta_{t'}d\theta_{t'}/\pi} \\
&= \sum_{m=0}^{1}\{\frac{d}{d\theta_t} < k,\theta_t|\}|m,\theta_t >< m,\theta_t|U_\theta(\theta_t)|j,\theta_a > \mathrm{e}^{-\mathrm{i}2(2k-1)\eta\int_{\theta_a}^{\theta_t}\theta_{t'}d\theta_{t'}/\pi} \\
&= -\sum_{m=0}^{1}\{< k,\theta_t|\frac{d}{d\theta_t}|m,\theta_t >\} < m,\theta_t|U_\theta(\theta_t)|j,\theta_a > \mathrm{e}^{-\mathrm{i}2(2k-1)\eta\int_{\theta_a}^{\theta_t}\theta_{t'}d\theta_{t'}/\pi}.
\end{aligned}\tag{G.3}$$

Using the relation, $< k,\theta_t|\frac{d}{d\theta_t}|m,\theta_t >= -(2k-1)\delta_{m,1-k}$, we obtain Eq.(3.17),

$$\begin{aligned}
\frac{d}{d\theta_t}\hat{a}_{k|j}(\theta_t) &= (2k-1) < 1-k,\theta_t|U_\theta(\theta_t)|j,\theta_a > \mathrm{e}^{-\mathrm{i}2(2k-1)\eta\int_{\theta_a}^{\theta_t}\theta_{t'}d\theta_{t'}/\pi} \\
&= (2k-1)\mathrm{e}^{-\mathrm{i}4(2k-1)\eta\int_{\theta_a}^{\theta_t}\theta_{t'}d\theta_{t'}/\pi}\hat{a}_{1-k|j}(\theta). \\
&= (2k-1)\mathrm{e}^{-\mathrm{i}2(2k-1)\eta(\theta^2-\theta_a^2)/\pi}\hat{a}_{1-k|j}(\theta).
\end{aligned}$$

For $j=1$ and $k=0,1$,

$$\frac{d}{d\theta}\hat{a}_{0|1}(\theta) = -\mathrm{e}^{\mathrm{i}2\eta(\theta^2-\theta_a^2)/\pi}\hat{a}_{1|1}(\theta), \tag{G.4}$$

$$\frac{d}{d\theta}\hat{a}_{1|1}(\theta) = \mathrm{e}^{-\mathrm{i}2\eta(\theta^2-\theta_a^2)/\pi}\hat{a}_{0|1}(\theta). \tag{G.5}$$

Using these equations,

$$\begin{aligned}
\frac{d^2}{d^2\theta}\hat{a}_{0|1}(\theta) &= -\frac{d}{d\theta}(\mathrm{e}^{\mathrm{i}2\eta(\theta^2-\theta_a^2)/\pi}\hat{a}_{1|1}(\theta)) \\
&= -(\frac{d}{d\theta}\mathrm{e}^{\mathrm{i}2\eta(\theta^2-\theta_a^2)/\pi})\hat{a}_{1|1} - \mathrm{e}^{\mathrm{i}2\eta(\theta^2-\theta_a^2)/\pi}\frac{d}{d\theta}\hat{a}_{1|1}(\theta) \\
&= -\mathrm{i}4\eta\theta/\pi\mathrm{e}^{\mathrm{i}2\eta(\theta^2-\theta_a^2)/\pi}\hat{a}_{1|1} - \hat{a}_{0|1}(\theta) \\
&= \mathrm{i}4\eta\theta/\pi\frac{d}{d\theta}\hat{a}_{0|1}(\theta) - a_{0|1}(\theta).
\end{aligned}\tag{G.6}$$

$\hat{a}_{0|1}(\theta_t)$ satisfies the following differential equation,

$$\frac{d^2}{d\theta_t^2}\hat{a}_{0|1}(\theta_t) - \mathrm{i}4\eta\theta/\pi\frac{d}{d\theta_t}\hat{a}_{0|1}(\theta_t) + \hat{a}_{0|1}(\theta_t) = 0. \tag{G.7}$$

We obtain Eq.(3.18) as a general solution of this differential equation,

$$\hat{a}_{0|1}(\theta) = c_1\mathrm{He}(-\mathrm{i}\frac{\pi}{4\eta},(-1)^{1/4}\theta\sqrt{\frac{2\eta}{\pi}}) + c_2\mathrm{F}_1(\mathrm{i}\frac{\pi}{8\eta},\frac{1}{2},\mathrm{i}\frac{2\theta^2\eta}{\pi})$$

where c_1 and c_2 are constants, He is a Hermite polynomial, and F_1 is a confluent hypergeometric function of the first kind [40]. They are generalized for complex parameters and complex variable.

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