

Analysis of finite-size effects in quantum thermodynamics of multiple
conserved quantities beyond i.i.d. regime

(複数保存量の量子熱力学における有限効果の独立同一分布を超えた解析)

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Abstract

In quantum thermodynamics, effects of finiteness of the baths have been less considered. In particular, there is no general theory which focuses on finiteness of the baths of multiple conserved quantities. Then, we investigate how the optimal performance of generalized heat engines with multiple quantities alters in response to the size of the baths. In the context of general theories of quantum thermodynamics, the size of the baths has been given in terms of the number of identical copies of a system, which does not cover even such a natural scaling as the volume. In consideration of the asymptotic extensivity, we deal with a generic scaling of the baths to naturally include the volume scaling. Based on it, we derive a bound for the performance of generalized heat engines reflecting finite-size effects of the baths, which we call fine-grained generalized Carnot bound. We also construct a protocol to achieve the optimal performance of the engine given by this bound. Finally, applying the obtained general theory, we deal with simple examples of generalized heat engines. 1D Ising spin chain model and a toy model of two-level particles illustrate strange behaviors of the finite-size effects. Another example is a heat engine with two baths composed of an ideal gas exchanging particles, where the volume scaling is applied. The result implies that the mass of the particle explicitly affects the performance of this engine with finite-size baths.

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Table 1.1: Regimes treated in conventional quantum thermodynamics. We fill in all the rest of regimes.

conserved quantities	i.i.d. scaling		Generic scaling	
	Thermodynamic limit	Finite-size effects	Thermodynamic limit	Finite-size effects
only energy	many (e.g. [2–4, 9])	[19]	other approaches [20, 21]	none
multiple	[12, 16]	none	none	none

1 Introduction

1.1 Motivation

Thermodynamics has succeeded in revealing the universal principles of nature since its origin by Carnot [1]. Carnot efficiency is given only by the temperatures of heat baths independently of other details of the systems. Coarse-grained perspective of extremely enormous systems enables such descriptions by a few number of quantities. On the other hand, it is ubiquitous in physics that effective theories alter in accordance with the scale. Researchers are now working on various scales of thermodynamics from microscopic to macroscopic. Recent explosion of studies on resource theories of quantum thermodynamics has worked out fine-grained thermodynamic laws of small systems [2–9]. Moreover, quantum thermodynamics of multiple conserved quantities including non-commutative observables has also been actively studied [10–16] recently. A primary system with multiple conserved quantities in thermodynamics is a system which exchanges the energy and the particle number with reservoirs (heat baths and particle baths), whose thermal state is described by the grand canonical ensemble. Jaynes [17, 18] further generalized thermodynamics for arbitrary multiple conserved quantities.

Although many studies [2–16] of quantum thermodynamics focused on the finiteness of the working substance of thermal machines, less studies has been done on the finite-size effects of the heat baths. Heat baths are treated as unboundedly available resources by the majority of conventional research. As pointed out by [19, 22], the baths should be treated as finite resources when the size of the baths is restricted during the thermodynamic process. For example, when the source and sink are given as mesoscopic systems, such a formulation is desired. Very recently, this topic attracts increasing attentions [19, 22–25]. In particular, Tajima and Hayashi [19] derived the asymptotic expansion of the optimal efficiency of heat engines with respect to the system-size n , the number of identical copies of the baths. In this expansion, since the first leading term expresses the optimal efficiency with thermodynamic limit, the second leading term expresses the finite-size effect appearing in the optimal efficiency. Although this type of argument is not common in quantum thermodynamics, it became very common in recent years in quantum and classical information theory [26–30], which is often called second order asymptotics. We can expect that the second leading term has similar importance in quantum thermodynamics.

Although the paper [19] was a first step to quantitative analysis of scale dependency in quantum thermodynamics, their analysis with finite-size baths is limited to the case when the energy is extracted from two heat bathes with different temperatures. In fact, there is no research on *finite-size baths of multiple conserved quantities* in quantum thermodynamics yet (Table 1.1). In an ordinary heat engine, only the energy transfer is involved. In contrast, when a thermal machine transfers multiple conserved quantities, we call it a generalized heat engine.

Many interesting systems involving multiple conserved quantities, e.g. electric batteries, biological processes, chemical reactions, etc, are possibly affected by finiteness of the baths. To investigate the

finite-size effects of generalized baths, we study how the optimal performance of generalized heat engines alters in response to the scale. For this purpose, we improve the second order asymptotics for multiple conserved quantities. That is, in the sense of second order asymptotics, we investigate the dependence of the performance of generalized heat engines on the baths' scale. We also give a simple protocol to achieve the optimal performance.

Next, we revisit 'scaling' in quantum thermodynamics. Most of the existing studies on quantum thermodynamics employ the identical and identically distribution (i.i.d.)-based scaling, where the baths are scaled by the number n of identical copies of the system. In general, the scaling of systems in nature is not necessarily given as the i.i.d.-scaling but rather in a more generic form, like the volume of the container including the gas, as has originally been treated in thermodynamics and statistical mechanics. Thus, the i.i.d.-scaling is quite constrained in general. In particular, to treat the change of the number of particles such as particle transport and chemical reactions, it is natural to use the scaling in terms of the 'volume' of the system. To extend the applicability of quantum thermodynamics to a wide range of natural objects, we establish a more general formulation of scaling beyond the i.i.d.-structure. Especially, we achieve it in consideration of the asymptotic extensivity (recently, Tajima et al. [20,21] independently took other approaches to non-i.i.d. based on the large deviation property to treat non-i.i.d. Gibbs states in thermodynamic limit). Based on such a generic scaling, we construct a protocol for a generalized heat engine under such a generalized scaling, which is novel even in thermodynamic limit (Table 1.1). As a typical example, we deal with a heat engine with two baths composed of ideal gas exchanging particles where the size of the baths is given by the volume. Applying our general theory, we calculate the finite-size effects on the optimal performance of this canonical example of a generalized heat engine.

Then, our results are roughly made up of two aspects: extension of the scaling of the baths to a generic manner, and generalization of the finite-size reservoir thermodynamics to multiple quantum conserved quantities, in terms of this generic scaling, which fills in untouched regimes (Table 1.1).

1.2 Overview

In this paper, we explicitly reveal the effects of the finiteness of the baths on the optimal performance of a generalized heat engine with multiple conserved quantities, even when they are not necessarily mutually commutative. Especially, we treat finiteness of the baths by the generic scaling parameter λ which can be discrete or even continuous. Instead of assuming the i.i.d. form scaling of the baths, we just impose the asymptotic extensivity on appropriate quantities with respect to the scaling parameter λ . The deviation from extensivity, because of the finiteness, may reflect the effects of the interactions and the boundary. Of course, the i.i.d.-scaling is also covered since the extensivity is trivially satisfied.

First of all, we focus on the bound on the performance (Sec. 3). To this end, we have to impose appropriate constraints on allowed operations. We have two ways to describe the battery system storing the extracted quantity: implicitly or explicitly [12]. Implicit-battery formulation just focuses on the operations on the bath $\mathcal{H}_{\text{Baths}}$ and working body \mathcal{H}_C , and describes the extracted quantity as the difference between their quantities before and after the operation so that the battery storing it is implicitly given outside of them. Explicit-battery formulation includes the battery system as an explicit quantum system \mathcal{H}_W so that we explicitly treat the whole system $\mathcal{H}_{\text{Baths}} \otimes \mathcal{H}_C \otimes \mathcal{H}_W$. Since the implicit-battery formulation describes a part of the whole dynamics, an operation in the implicit-battery formulation corresponds to many operations in the explicit-battery formulations in general. In the derivation of an upper bound of the performance, as weak as possible constraints are preferable for wide applicability. That is, a necessary condition for permissible operation is sufficient to impose. In this sense, we derive a bound under the appropriate implicit-battery formulation (Sec. 4.2). The recent paper [12] describes an operation in the

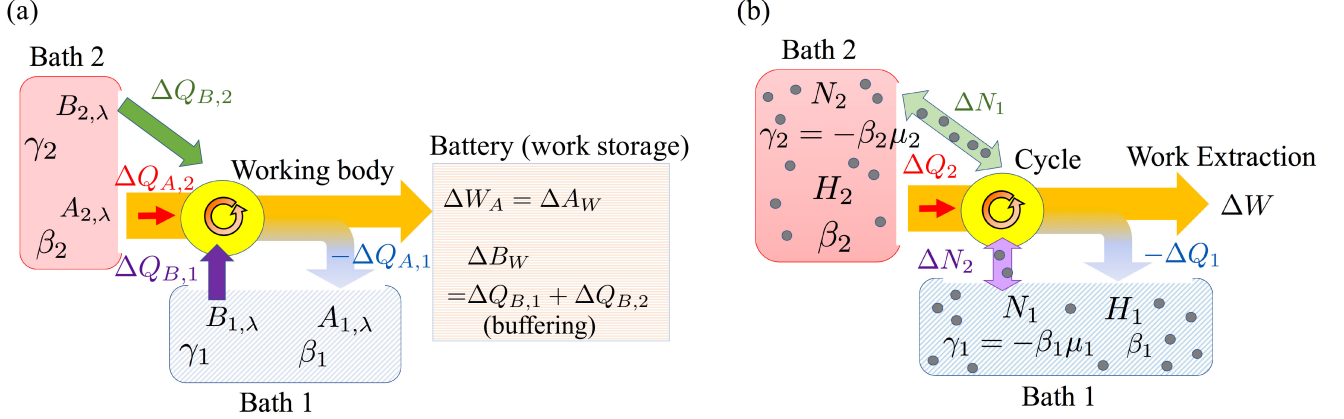


Figure 1.1: (a) Schematic picture of the model of generalized heat engines with multiple conserved quantities. Each bath has two kinds of quantities $A_{i,\lambda}$ and $B_{i,\lambda}$, which are, for example, energy, particle number, x -component of angular momentum, etc. We assume that generalized inverse temperatures β_i and γ_i conjugate to $A_{i,\lambda}$ and $B_{i,\lambda}$ respectively are assigned to each bath. GCB implies that in extraction of Quantity A through the supply $\Delta Q_{A,2}$ from Bath 2, “waste heat” $-\Delta Q_{A,1}$ to Bath 1 can be reduced by the supplies $\Delta Q_{B,1}$ and $\Delta Q_{B,2}$ of quantity B from the two baths. The finite-size effects in FGCB reflect the canonical correlations of the baths’ quantities. Of course, we can consider a generalized heat pump in the same way by running it oppositely. (b) Schematic picture of a heat engine with particle transport, which is a primary example of a generalized heat engines. We treat it in detail in Sec. 9.4. This engine extracts work through exchanging heat energy and identical particles with two baths. In this case, Quantity A is the energy, and B is the number of identical particles. Each bath i has corresponding Hamiltonian $H_{i,\lambda}$ and the particle number $N_{i,\lambda}$. Ordinary inverse temperature β_i conjugate to $H_{i,\lambda}$ is assigned to each bath. The generalized inverse temperature γ_i conjugate to the particle number $N_{i,\lambda}$ is given as $\gamma_i = -\beta_i\mu_i$, where μ_i is the chemical potential of Bath i . Waste heat can be reduced by compensating it by particle transport. Finite-size effects in the optimal performance reflect the canonical correlation of $H_{i,\lambda}$ and $N_{i,\lambda}$, as well as the fluctuation of $H_{i,\lambda}$ and $N_{i,\lambda}$.

implicit-battery formulation as a unitary operation on $\mathcal{H}_{\text{Baths}} \otimes \mathcal{H}_C$, corresponding to the dynamics of the system driven by semi-classical external field. However, since the reduced dynamics of $\mathcal{H}_{\text{Baths}} \otimes \mathcal{H}_C$ tracing out the battery \mathcal{H}_W is not unitary without approximation in general, we include wider class of operations as operations with implicit battery: unital completely positive and trace preserving (CPTP)-maps [31]. The unitalness is equivalent to non-decreasing of von Neumann entropy, which is analogous to adiabaticity with the battery in macroscopic thermodynamics. Furthermore, as the reduced dynamics from the operations with an explicit battery, the unitalness indeed follows from translational symmetry of the battery [12, 31, 32], which is imposed to guarantee that no hidden heat-like transfer cheatingly improves the performance. Since we consider the working body executing a cycle, we also impose the cyclicity with respect to \mathcal{H}_C .

Let us consider a generalized heat engine with two baths, namely Baths 1 and 2, of two kinds of conserved quantities, namely Quantities A and B , for simplicity (Fig. 1.1 (a)). For our formulation, the role of Quantities A and B are essentially the same. Thus, we focus on the bound on the extraction ΔW_A of Quantity A without loss of generality. We can choose A and B as arbitrary conserved quantities. For example, one may choose the energy as Quantity A to focus on the work extraction, or one may choose the particle number as Quantity A to focus on the extraction of the number of particles. Heat engine with particle transport (Fig 1.1 (b)) is a canonical example of the generalized heat engine. Our objective is the upper bound on the extraction ΔW_A of Quantity A by a cyclic process where the generalized heat $\Delta Q_{A,i}$ of Quantity A and $\Delta Q_{B,i}$ of quantity B are absorbed from Bath i (Fig. 1.1 (a)). Under the implicit-battery formulation, the second law for multiple conserved quantities [12] immediately implies the following upper bound for the extraction ΔW_A :

$$\Delta W_A \leq \left(1 - \frac{\beta_2}{\beta_1}\right) \Delta Q_{A,2} - \sum_{i=1}^2 \frac{\gamma_i}{\beta_1} \Delta Q_{B,i}, \quad (1.1)$$

where the baths are initially in the generalized thermal state at the respective generalized inverse temperatures β_i and γ_i corresponding to Quantities A and B of Bath i (For the definitions of generalized thermal state and generalized inverse temperature, see Definition 2.1).

Remark 1.1. *This bound does not include $\Delta Q_{A,1}$ since ΔW_A is determined if we fix both $\Delta Q_{A,1}$ and $\Delta Q_{A,2}$. Rather $\Delta Q_{A,1}$ is constrained when the others $\Delta Q_{A,2}$, $\Delta Q_{B,1}$ and $\Delta Q_{B,2}$ are given. The bound (1.1) is obtained through this constraint. This situation is similar to the ordinary Carnot bound, where the upper bound for the work extraction ΔW is given in response to the endothermic heat ΔQ_h from the hot bath:*

$$\Delta W \leq \left(1 - \frac{\beta_h}{\beta_c}\right) \Delta Q_h, \quad (1.2)$$

where β_h and β_c are the inverse temperatures of the hot and the cold baths, respectively.

We call the bound (1.1) the generalized Carnot bound (GCB) since this is a straightforward generalization of the Carnot bound, which has a similar structure depending only on the generalized inverse temperatures. However, because of finite-size effects, this bound is never achievable unless thermodynamic limit is taken.

Throughout the paper, we assume that the generalized heat is small enough relative to the scale (see (3.7)) because the baths' state should be unchanged in thermodynamic limit. Then, by incorporating finite-size effects into GCB, our first main result is the following inequality, which we call fine-grained

generalized Carnot bound (FGCB) (Sec. 3.3 Theorem 3.1):

$$\begin{aligned} \Delta W_A \lesssim & \left(1 - \frac{\beta_2}{\beta_1}\right) \Delta Q_{A,2} - \sum_{i=1}^2 \frac{\gamma_i}{\beta_1} \Delta Q_{B,i} \\ & - C_{AA} \frac{\Delta Q_{A,2}^2}{\lambda} - \sum_{i=1}^2 C_{AB}^i \frac{\Delta Q_{A,2} \Delta Q_{B,i}}{\lambda} - \sum_{i,j=1}^2 C_{BB}^{i,j} \frac{\Delta Q_{B,i} \Delta Q_{B,j}}{\lambda}. \end{aligned}$$

The leading terms are the same as the GCB, corresponding to thermodynamic limit. The next leading terms reflect the largest finite-size effect, which is indeed always negative, so that FGCB does not exceed GCB. This finite-size effect represents the decrease of the performance caused by the non-negligible disturbance to the state of the baths due to their finiteness. FGCB gives us the guideline for relieving such drawback. The canonical correlations of the baths' observables are included in the coefficients $C_{AA}, C_{AB}^i, C_{BB}^{i,j}$ ((3.11)-(3.13)) of the second leading terms. Thus, correlations reflecting non-commutativity of the conserved quantities explicitly affects the performance, quite differently from thermodynamic limit described by GCB. Especially, correlation between Bath 1 and 2 is also reflected. We should consider such correlation structures of the baths to design the engine with finite-size baths.

Work extraction from spin chains (Sec. 9.2) and a spin- $\frac{1}{2}$ bath (Sec. 9.3) as generalized heat engines simply illustrate the behavior of the second leading term. Furthermore, we consider the heat engine with baths composed of an ideal gas exchanging particles whose size is given by the volume of the container in Sec. 9.4, as a more physical example (Fig. 1.1 (b)). Although it is so famous canonical example, this is the first time to explicitly calculate the finite-size effects on the optimal performance of this kind of heat engine.

It is also important to show how the bound can be achieved. Hence, we construct a protocol to achieve the FGCB (Sec. 4). In construction of the protocol, we should carefully avoid any hidden heat source which may cheatingly improve apparent performance of the engine, because the definition of work-like transfer of each quantity is ambiguous in quantum thermodynamics. Thus, we have to explicitly treat the battery to show the achievability of optimal performance in FGCB. For an explicit treatment, in addition to the conservation laws and cyclicity of the working body, we should restrict the battery to really work just as a battery but not as a 'cold reservoir'. A reasonable condition is the 'no-cheating' condition [12,32,33], which restricts the protocol to be independent of the state of the battery. In this way, it is guaranteed that the battery itself can not be used cheatingly as an entropy sink. In this sense, any exchange of the quantities with the battery does not improve the performance cheatingly as hidden heat-like transfer. We consider a realization of the battery with continuous spectrum to satisfy this no-cheating condition, and finally construct the protocol with the explicit battery. Furthermore, there are two types of conservation laws, the strict and average conservation laws [12,34]. The strict conservation requires that each quantity commutes with the dynamics, while the average conservation requires only the conservation of its average value. When the observables representing the conserved quantities are commutative, we construct a protocol satisfying the strict conservation. However, for the non-commuting case, it is not easy to construct such a protocol. Instead of this requirement, we construct a protocol satisfying just the average conservation law as in [12,32]. As pointed out in [34], coherence may be indefinitely needed to realize a protocol satisfying just the average conservation. However, it is also pointed out in [34] that considering resource of coherence appropriately [35], we have a possibility to transform a protocol satisfying the average conservation law to a protocol satisfying the strict conservation law.

FGCB is "formally" attained by the final thermal state at the ideal final inverse temperature defined by (3.23)-(3.26) in Sec. 3.3. However, this final thermal state is not realizable from the initial thermal

state by any protocol in general. Instead, our protocol makes the final state very close to the thermal state at the ideal final inverse temperature. To show that our protocol indeed achieves FGCB (Theorems 4.1, 4.2), we impose additional assumptions (Assumption 4.1 and (4.16)). Assumption 4.1 is a stronger version of the asymptotic extensivity which guarantees small enough deviation from the extensivity. The condition (4.16) requires large enough generalized heat. Finally, under these assumptions, we show that our protocol achieves the equality in FGCB asymptotically by making use of information geometric structure of thermal states. A similar idea was given for an ordinary heat engine in [36].

1.3 Organization

This paper is organized as follows. In Sec. 2, we present the setup for our analysis. At first, we introduce the generalized heat engine and the generalized thermal state in Sec. 2.1. Next, we bring in a scaling of the baths based on the asymptotic extensivity in Sec. 2.2 beyond the identical and independent distributions. Sec. 3 is devoted to show our first main result fine-grained generalized Carnot bound (FGCB). The implicit-battery formulation is introduced to deal with the bound on the optimal performance in Sec. 3.1. In Sec. 3.2, we review the second law of thermodynamics with multiple conserved quantities, and introduce the generalized Carnot bound (GCB). FGCB is shown in Sec. 3.3. We construct the optimal protocol to show the tightness of FGCB in Sec. 4. Firstly, we construct an operation with implicit battery in Sec. 4.1. Then, in Sec. 4.3, we extend the implicit-battery protocol to the explicit-battery formulation which is introduced in Sec. 4.2. Next, we show the statement of the theorem (Theorem 4.1) of asymptotic optimality of our protocol in Sec. 4.4. We also show the outline of its proof and prepare a lemma (Lemma 4.1) in Sec. 4.4. The proof is completed in Sec. 8 after preparing necessary lemmas in Sec. 5-7. We extend the construction of our protocol to non-commutative quantities in Sec. 4.5 under the average conservation laws. A proof of its optimality (Theorem 4.2) is also shown in Sec. 8. To prove Theorems 4.1 and 4.2, we estimate the order of the relative entropy between the constructed state and an ideal state. Extending the central limit theorem to our generic scaling in Sec. 5, we apply the strong large deviation to the number of states and obtain its asymptotic expansion (Lemma 6.1) in Sec. 6. Then, we obtain the desired estimation in Sec. 7 by applying Lemma 6.1. As mentioned above, we prove Theorems 4.1 and 4.2 in Sec. 8 by applying the estimation in Sec. 7. We apply our general theory to some examples in Sec. 9. Finally, the conclusion is in Sec. 10. In Appendix A, we provide some basic aspects of information geometry which is used in the proof of Lemma 4.1.

2 Setup

2.1 Heat engine with generalized thermal baths

We consider a generalized heat engine to extract arbitrary quantities composed of multiple baths and a working body as Fig. 1.1. We denote the Hilbert space of the system composed of all the baths by $\mathcal{H}_{\text{Baths}}$. The working body is supposed to execute the cyclic process, which is denoted by \mathcal{H}_C . In addition, we denote the battery system to store the extracted quantities by \mathcal{H}_W . All these Hilbert spaces depend on the scale parameter λ , though we abbreviate the notation.

The system $\mathcal{H}_{\text{Baths}}$ consists of two generalized baths, Baths 1 and 2, each of which exchanges two conserved quantities (Quantities A and B) with the working body and the battery. We set both numbers of the conserved quantities and the baths as two since our results are essentially the same for general multiple baths and quantities. It is straightforward to generalize our results to the case of arbitrary number of the baths with arbitrarily many conserved quantities. Especially, for only one bath with two

quantities ($m = 1, K = 2$), it is sufficient to omit one of the baths (see an example in Appendix 9.3). For example, each conserved quantity A or B may stand for energy, particle number, x -component of the angular momentum, etc. We denote Quantities A and B of Bath i ($i = 1, 2$) with the scale λ by $A_{i,\lambda}$ and $B_{i,\lambda}$ respectively. Then, $\mathcal{H}_{\text{Baths}}$ has the observables $X_{j,\lambda}$ ($j = 1, 2, 3, 4$), where $X_{1,\lambda} = A_{1,\lambda}$, $X_{2,\lambda} = A_{2,\lambda}$, $X_{3,\lambda} = B_{1,\lambda}$, $X_{4,\lambda} = B_{2,\lambda}$. In general, we do not assume commutativity of $X_{j,\lambda}$'s. Especially, quantities from the different baths (e.g. $A_{1,\lambda}$ and $A_{2,\lambda}$) can be correlated.

For simplicity, we assume that the dimension $d_\lambda > 4$ of the baths' Hilbert space $\mathcal{H}_{\text{Baths}}$ is finite but depending on the scale λ . In addition, we assume that $X_{j,\lambda}$ ($j = 1, 2, 3, 4$) and the identity I are linearly independent as real vectors. Otherwise, the relation $X_{j,\lambda} = \sum_{k \neq j} a_k X_{k,\lambda} + aI$ holds for a j with some real numbers a_k and a , which implies that $X_{j,\lambda}$ is a redundant quantity since it is just a linear combination of the other quantities plus a constant a . Thus, we assume this linear independence. Note that our scaling of the baths is different from the conventional one where the baths consist of many identical copies of a system. We just assume the asymptotic extensivity of the baths' quantities with respect to this generic scale parameter λ , which can even be continuous, as we discuss in detail in the next subsection. Suppose that the initial state of the baths is the generalized thermal state with the associated generalized inverse temperatures θ^j conjugate to $X_{j,\lambda}$ ($j = 1, 2, 3, 4$). We also denote the generalized inverse temperatures associated with $A_{i,\lambda}$ and $B_{i,\lambda}$ by β_i and γ_i respectively to emphasize which quantity and bath correspond to each generalized inverse temperature. The generalized thermal state and generalized inverse temperature are defined as follows:

Definition 2.1 (Generalized thermal state [12, 15, 18]). *Let $\mathcal{Z}(\boldsymbol{\theta}) := \text{tr} e^{-\sum_{j=1}^4 \theta^j X_{j,\lambda}}$ be the generalized partition function with $\boldsymbol{\theta} = (\theta^1, \theta^2, \theta^3, \theta^4)$, the generalized thermal state at a generalized inverse temperature $\boldsymbol{\theta}$ is*

$$\tau_{\boldsymbol{\theta}}^{(\lambda)} := \frac{e^{-\sum_{j=1}^4 \theta^j X_{j,\lambda}}}{\mathcal{Z}(\boldsymbol{\theta})} = \frac{e^{\sum_{i=1}^2 (-\beta_i A_{i,\lambda} - \gamma_i B_{i,\lambda})}}{\mathcal{Z}(\boldsymbol{\theta})}. \quad (2.1)$$

As a function of the inverse temperature coordinate $\boldsymbol{\theta}$, we define the generalized free entropy (also known as the Massieu potential) $\phi_\lambda(\boldsymbol{\theta}) := \log \mathcal{Z}(\boldsymbol{\theta})$ of the thermal state.

The ordinary grand canonical state is a typical example of the generalized thermal state. It is the thermal state of the system exchanging the particles as well as the energy with the large reservoir. The particle number and energy of the total system are conserved. In this case, observables are $X_{1,\lambda} = H_{1,\lambda}$, $X_{2,\lambda} = H_{2,\lambda}$, $X_{3,\lambda} = \mathcal{N}_{1,\lambda}$, and $X_{4,\lambda} = \mathcal{N}_{2,\lambda}$, where $H_{j,\lambda}$ and $\mathcal{N}_{j,\lambda}$ are the Hamiltonian and the particle number operator of Bath j , respectively. The generalized inverse temperatures are composed of the inverse temperature β_i and the chemical potential μ_i of each Bath i as $\theta^i = \beta_i$, $\theta^{i+2} = -\beta_i \mu_i$ ($i = 1, 2$). In the same way as the grand canonical state, the state given by Definition 2.1 was shown to be the thermal state of the system exchanging non-commuting charges with a large reservoir [15]. In this sense, we consider a small part of the large reservoir as our finite-size bath.

We regard the average value as the extracted amount of each quantity in the same way as [12, 32]. Another formulation is so-called single-shot thermodynamics [3, 24]. This formulation of deterministic work is quite different from work extraction to macroscopic systems at the point that its battery is a wit, which is a two level system with a predetermined energy gap. We rather focus on non-deterministic transfer of the quantity.

To derive the universal optimal performance, we consider general dynamics of the generalized heat engine (Fig. 1.1 (a)) where the conservation law among the total system including the battery for every conserved quantity. However, there are two kinds of conservation laws, the strict and average conservation

laws [12, 34]. The strict conservation requires that each quantity commutes with the dynamics, while the average conservation requires only the conservation of its average value. It is important to distinguish them when we consider the allowed operations on the whole system $\mathcal{H}_{\text{Baths}} \otimes \mathcal{H}_C \otimes \mathcal{H}_W$ in Sec. 4.2 and 4.5. Since the average conservation follows from the strict conservation, under both conservation laws, the average value of each quantity is exchanged between the baths and the battery through the cyclic process by the working body. Hence, the sums $-\sum_{i=1} \Delta A_{i,\lambda}$ and $-\sum_{i=1} \Delta B_{i,\lambda}$ of the differences in the average values of Quantities A and B are respectively stored in the battery.

2.2 Extensivity of baths

We consider the behavior of the heat engine when λ grows large under the fixed initial inverse temperature $\boldsymbol{\theta} = \boldsymbol{\theta}_0$, which generalizes the consideration of grand-canonical type ensemble. The free entropy ϕ_λ is almost the same as the free energy, but rather more natural for dealing with multiple conserved quantities [12]. It is the generating function of the physical quantities. The first derivatives are the expectation value

$$\eta_{\lambda,j}(\boldsymbol{\theta}) := -\frac{\partial \phi_\lambda}{\partial \theta^j}(\boldsymbol{\theta}) = \text{tr } X_{j,\lambda} \tau_{\boldsymbol{\theta}}^{(\lambda)}. \quad (2.2)$$

This still holds for non-commutative quantities. As common in information geometry [37], $\eta_{\lambda,i}(\boldsymbol{\theta})$ can be regarded as a component of the dual coordinate of $\boldsymbol{\theta}$ composed of the expectation values (see Appendix A.2)

$$\boldsymbol{\eta}_\lambda(\boldsymbol{\theta}) := (\eta_{\lambda,1}(\boldsymbol{\theta}), \eta_{\lambda,2}(\boldsymbol{\theta}), \eta_{\lambda,3}(\boldsymbol{\theta}), \eta_{\lambda,4}(\boldsymbol{\theta})) = (\text{tr } A_{1,\lambda} \tau_{\boldsymbol{\theta}}^{(\lambda)}, \text{tr } A_{2,\lambda} \tau_{\boldsymbol{\theta}}^{(\lambda)}, \text{tr } B_{1,\lambda} \tau_{\boldsymbol{\theta}}^{(\lambda)}, \text{tr } B_{2,\lambda} \tau_{\boldsymbol{\theta}}^{(\lambda)}). \quad (2.3)$$

The second derivatives form the Fisher information matrix composed of the canonical correlation

$$J_{\lambda,ij}(\boldsymbol{\theta}) := \frac{\partial^2 \phi_\lambda}{\partial \theta^i \partial \theta^j}(\boldsymbol{\theta}) = \int_0^1 ds \text{tr} \left[\left(\tau_{\boldsymbol{\theta}}^{(\lambda)} \right)^{1-s} X_{i,\lambda} \left(\tau_{\boldsymbol{\theta}}^{(\lambda)} \right)^s X_{j,\lambda} \right] - \eta_{\lambda,i}(\boldsymbol{\theta}) \eta_{\lambda,j}(\boldsymbol{\theta}). \quad (2.4)$$

The canonical correlation reduces to the covariance for commutative observables. In the same way, the third derivatives correspond to the skewness. These statistical quantities are expected to be extensive in thermodynamics. Thus, it is natural to assume that the free entropy and its derivatives are asymptotically extensive. More precisely, we impose the following:

Assumption 2.1. *There exists an asymptotic density $\phi(\boldsymbol{\theta})$ of the free entropy $\phi_\lambda(\boldsymbol{\theta})$ as a smooth function satisfying the following condition. As $\lambda \rightarrow \infty$, the free entropy ϕ_λ asymptotically satisfies*

$$\phi_\lambda(\boldsymbol{\theta}) = \lambda \phi(\boldsymbol{\theta}) + o(\lambda), \quad (2.5)$$

uniformly on a neighborhood of $\boldsymbol{\theta}_0$. Moreover, up to the third-order partial derivatives of ϕ_λ satisfies the similar condition uniformly on a neighborhood of $\boldsymbol{\theta}_0$:

$$\left(\frac{\partial}{\partial \theta^{i_1}} \right)^{l_1} \left(\frac{\partial}{\partial \theta^{i_2}} \right)^{l_2} \left(\frac{\partial}{\partial \theta^{i_3}} \right)^{l_3} \phi_\lambda(\boldsymbol{\theta}) = \left(\frac{\partial}{\partial \theta^{i_1}} \right)^{l_1} \left(\frac{\partial}{\partial \theta^{i_2}} \right)^{l_2} \left(\frac{\partial}{\partial \theta^{i_3}} \right)^{l_3} \lambda \phi(\boldsymbol{\theta}) + o(\lambda) \quad (2.6)$$

for all integers l_1, l_2, l_3 with $0 < l_1 + l_2 + l_3 \leq 3$, $i_1, i_2, i_3 \in \{1, 2, 3, 4\}$. The matrix $(\frac{\partial^2 \phi}{\partial \theta^i \partial \theta^j}(\boldsymbol{\theta}))_{ij}$ is assumed to be full rank.

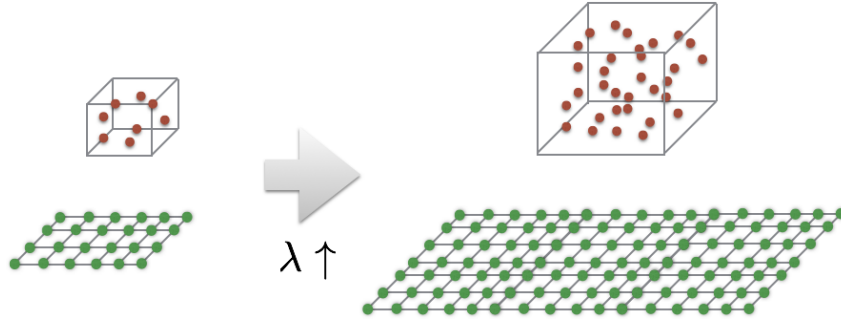


Figure 2.1: Homothetic scaling of the baths. Even if the dimensions of the systems are different from each other, it is sufficient to put λ as a dimensionless scaling parameter by defining the unit size of each system.

This asymptotic extensivity is widely expected as long as the system is thermodynamic in large scale since the free entropy should be an extensive quantity as is the case with the free energy. Especially, the asymptotic extensivity of the free energy was rigorously proved for Hamiltonians with short range interaction [38], though any similar theorem is not known for the general multiple conserved quantities. The asymptotic extensivity (2.6) of the derivatives of the free entropy was not generically proved even for Hamiltonian in [38]. However, its validity is expected for usual systems since the derivatives correspond to extensive quantities in thermodynamic limit, such as the expectation values, fluctuations, and the statistical moments of the extensive quantities¹. In fact, Assumption 2.1 is verified for some examples in Sec. 9. It trivially holds for the i.i.d. scaling. A simple example of non-i.i.d. scaling with the asymptotic extensivity is a spin chain (Sec. 9.2). Furthermore, it is also satisfied by an ideal gas in the container (Sec. 9.4), where the volume is the scaling parameter.

In (2.5), $\phi(\boldsymbol{\theta})$ stands for the asymptotic density of the free entropy in the sense that $\phi(\boldsymbol{\theta}) = \lim_{\lambda \rightarrow \infty} \phi_\lambda(\boldsymbol{\theta})/\lambda$. The first derivatives $\eta_i(\boldsymbol{\theta}) := -\frac{\partial \phi}{\partial \theta^i}(\boldsymbol{\theta})$ and the second derivatives $g_{ij}(\boldsymbol{\theta}) := \frac{\partial^2 \phi}{\partial \theta^i \partial \theta^j}(\boldsymbol{\theta})$ of $\phi(\boldsymbol{\theta})$ also correspond to the asymptotic densities of the expectation values and canonical correlations, respectively, as seen from another expressions for them:

$$\eta_{\lambda,i}(\boldsymbol{\theta}) = \lambda \eta_i(\boldsymbol{\theta}) + o(\lambda), \quad (2.7)$$

$$J_{\lambda,ij}(\boldsymbol{\theta}) = \lambda g_{ij}(\boldsymbol{\theta}) + o(\lambda). \quad (2.8)$$

Thus, Assumption 2.1 coincides with the existence of the asymptotic density of each extensive quantity, in other words.

Here, we consider just one scaling parameter, but not as many parameters as the baths. That is, we fix the ratio between the sizes of the baths Fig. 2.1. Note that this scaling is applicable even if baths contain different dimensional systems or systems with different measures of their sizes by defining the unit size of each system. For example, consider the case where one bath is a two-dimensional system and the other is of three-dimensional, whose sizes are scaled by their area S and volume V respectively. Then, defining the unit area s_0 and volume v_0 , we consider the scaling $S = \lambda s_0$ and $V = \lambda v_0$ by the dimensionless parameter λ . In this case, the difference in their dimensionality is putted on their ‘ratio’ v_0/s_0 whose dimension is the length.

¹Especially, explicit assurance of the asymptotic extensivity of the third-derivatives in Assumption 2.1 is needed for our main analysis in Sec. 3.3, where we use it to verify the order of residual terms in fine-grained generalized Carnot bound to be negligible.

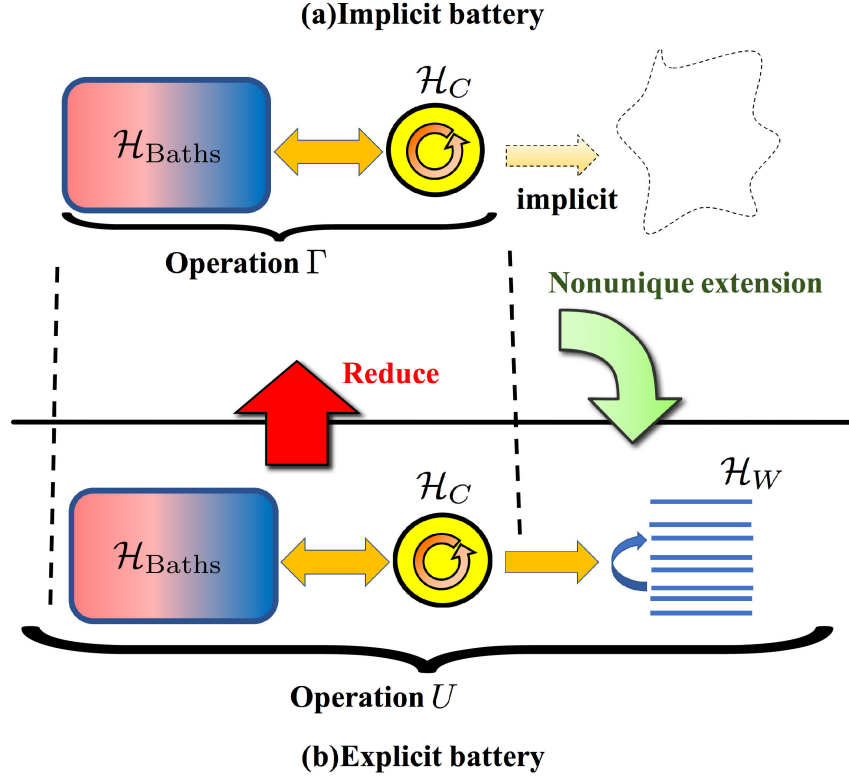


Figure 3.1: Schematic of (a) implicit-battery formulation and (b) explicit-battery formulation. An explicit-battery formulation is reduced to the corresponding implicit-battery formulation by tracing out \mathcal{H}_W , while extension from an implicit-battery formulation to some explicit-battery formulation is not unique.

In order to apply our analysis to a generalized heat engine, all we have to check is the existence of the scaling λ satisfying this property.

The last statement guarantees independence of the observables. More precisely, the expectation values of the observables can take any combinations under sufficiently large λ , since the Fisher information matrix $(\frac{\partial^2 \phi_\lambda}{\partial \theta^i \partial \theta^j}(\boldsymbol{\theta}))_{ij}$ is the same as the Jacobian matrix of the transformation of the variable from $\boldsymbol{\theta}$ to the expectation value.

3 Generalized Carnot bound for generalized work extraction with finite-size effects

3.1 Operations with implicit battery

There are two formulations of operations, the implicit-battery and the explicit-battery formulations (Fig. 3.1). The former focuses on the operations only on $\mathcal{H}_{\text{Baths}} \otimes \mathcal{H}_C$, so that the extracted amount of each quantity is stored in the implicitly existing battery outside of $\mathcal{H}_{\text{Baths}} \otimes \mathcal{H}_C$. The latter explicitly treats the operations on the whole system $\mathcal{H}_{\text{Baths}} \otimes \mathcal{H}_C \otimes \mathcal{H}_W$ under the conditions mentioned in Sec. 2.1. Macroscopic thermodynamics usually employs the implicit-battery formulation since the work is clearly defined and the functionality of the battery system is obvious. However, in quantum thermody-

namics, the definition of the work-like transfer of each quantity itself is ambiguous, and it is non-trivial to verify that there is no heat-like transfer with the battery, even in consideration of thermodynamic limit [12, 32, 39]. Thus, an implicit-battery operation has no clear meaning as a thermodynamic process, unless it is extended to an operation in an appropriate explicit-battery formulation. Such an extension to the explicit-battery formulation is nonunique in general. On the other hand, applicability of the upper bound on the extraction becomes wider as we derive it under as weak conditions as possible. Therefore, in our derivation of the FGCB, we focus on the implicit-battery operations on $\mathcal{H}_{\text{Baths}} \otimes \mathcal{H}_C$ which satisfy appropriate necessary conditions for being extended to an explicit-battery operation. We consider a concrete explicit formulation in Sec. 4.2 to construct the operation to achieve FGCB.

One way of the implicit-battery formulation is to restrict the operations to be unitary [12]. However, this restriction does not work because the state transitions are not guaranteed to be described by some unitary operation due to the interaction with the battery [31]. Indeed, the reduced operations on $\mathcal{H}_{\text{Baths}} \otimes \mathcal{H}_C$ are written as completely positive and trace preserving (CPTP)-maps in general. Thus, we impose the unitalness $\Gamma(I_{\text{Baths},C}) = I_{\text{Baths},C}$ on implicit-battery operations Γ on $\mathcal{H}_{\text{Baths}} \otimes \mathcal{H}_C$, which is equivalent to non-decreasing of von Neumann entropy. Here, $I_{\text{Baths},C}$ is the identity of $\mathcal{H}_{\text{Baths}} \otimes \mathcal{H}_C$. The unitalness is reasonable as a necessary condition because not only non-decreasing of von Neumann entropy corresponds to adiabaticity in the macroscopic thermodynamics but also the unitalness is actually derived from another reasonable condition on explicit-battery formulations. We impose that the global unitary operations in the explicit-battery formulation commute with all the translation operators on the battery (Sec. 4.2) as in [12, 31, 32]. As a natural situation, we consider the case where we cannot control the initial state on the battery and observe only the translation of the battery [32]. In order that the generalized heat engine works properly, we need such translational symmetry for the battery. In fact, the translational symmetry of the battery implies the unitalness of the reduced dynamics [12, 31, 32]. Hence, the unitalness is believed to be necessary in consideration of the performance of generalized heat engines. The cyclicity $\text{tr}_{\mathcal{H}_{\text{Baths}}} \Gamma(\tau_{\theta}^{(\lambda)} \otimes \rho_C) = \rho_C$ of the working body \mathcal{H}_C is also required. In this way, FGCB is applicable whenever the 'explicit' dynamics reduces to a unital channel on $\mathcal{H}_{\text{Baths}} \otimes \mathcal{H}_C$ with the cyclicity. Note that the cyclicity can depend on the initial state ρ_C of \mathcal{H}_C , so that ρ_C can be used as a catalyst to enlarge the class of possible operations on $\mathcal{H}_{\text{Baths}}$.

In summary, we employ the following operations in the implicit-battery formulation here:

Definition 3.1 (Operations in the implicit-battery formulation). *Allowed operations in the implicit-battery formulation are CPTP maps Γ on $\mathcal{H}_{\text{Baths}} \otimes \mathcal{H}_C$ which satisfies the following:*

A1. *Unitalness:*

$$\Gamma(I_{\text{Baths},C}) = I_{\text{Baths},C}. \quad (3.1)$$

A2. *Cyclicity of the engine:*

$$\text{tr}_{\mathcal{H}_{\text{Baths}}} \Gamma(\tau_{\theta}^{(\lambda)} \otimes \rho_C) = \rho_C. \quad (3.2)$$

3.2 Second law and the generalized Carnot bound in thermodynamic limit

Since operations are given as unital CPTP maps on $\mathcal{H}_{\text{Baths}} \otimes \mathcal{H}_C$ with the cyclicity, we have

$$S(\rho'_{\text{Baths}}) + S(\rho_C) \geq S(\Gamma(\tau_{\theta}^{(\lambda)} \otimes \rho_C)) \geq S(\tau_{\theta}^{(\lambda)} \otimes \rho_C) = S(\tau_{\theta}^{(\lambda)}) + S(\rho_C) \quad (3.3)$$

from the subadditivity of the von Neumann entropy. Therefore, the von Neumann entropy $S(\rho'_{\text{Baths}})$ of the final state $\rho'_{\text{Baths}} := \text{tr}_{\mathcal{H}_C} \Gamma(\tau_{\theta_0}^\lambda \otimes \rho_C)$ of the bath system satisfies

$$S(\rho'_{\text{Baths}}) \geq S(\tau_{\theta_0}^\lambda). \quad (3.4)$$

Thus, the relation $\Delta S := S(\rho'_{\text{Baths}}) - S(\tau_{\theta_0}^\lambda) = \sum_{i=1}^2 (\beta_i \Delta A_{i,\lambda} + \gamma_i \Delta B_{i,\lambda}) - D(\rho'_{\text{Baths}} \| \tau_{\theta_0}^{(\lambda)})$ yields the following second law of thermodynamics [12]:

$$\sum_{i=1}^2 (\beta_i \Delta A_{i,\lambda} + \gamma_i \Delta B_{i,\lambda}) \geq D(\rho'_{\text{Baths}} \| \tau_{\theta_0}^{(\lambda)}), \quad (3.5)$$

where $\Delta A_{i,\lambda} := \text{tr} A_{i,\lambda} (\rho'_{\text{Baths}} - \tau_{\theta_0}^{(\lambda)})$ and $\Delta B_{i,\lambda} := \text{tr} B_{i,\lambda} (\rho'_{\text{Baths}} - \tau_{\theta_0}^{(\lambda)})$ are the amounts of difference of $A_{i,\lambda}$ and $B_{i,\lambda}$ respectively, and $D(\rho \| \sigma) := \text{tr} \rho (\log \rho - \log \sigma)$ is the relative entropy between states ρ and σ .

As pointed out in [12], the relation (3.5) implies the trade-off relation between the amounts of extraction of quantities, instead of a constraint for each single quantity. Now, as a natural extension of the formulation of the ordinary Carnot bound, we formulate the generalized Carnot bound (GCB) for the extraction of Quantity A , without loss of generality. We call $\Delta Q_{A,i} := -\Delta A_{i,\lambda}$ and $\Delta Q_{B,i} := -\Delta B_{i,\lambda}$ the generalized heat. The extraction of A is defined as $\Delta W_A := \Delta Q_{A,1} + \Delta Q_{A,2}$ in the implicit-battery formulation. This definition is based on the conservation of the average value of the quantity. Though there are the strict and average conservation laws on the whole system in the explicit-battery formulation, the conservation of the average values is satisfied for both cases as mentioned in Sec. 2.1. Thus, both the strict and average conservation laws meet this definition of the work extraction in the implicit-battery formulation. The sum $\Delta B_{1,\lambda} + \Delta B_{2,\lambda}$ of the differences in quantity B does not have to vanish. The amount $\Delta Q_{B,1} + \Delta Q_{B,2}$ is stored as the gain or lose of the average value of quantity B of the battery in the same way, which may be regarded as the extraction of the other quantity or a ‘buffer’ to extract Quantity A .

Then, the relations (3.5) and $D(\rho'_{\text{Baths}} \| \tau_{\theta_0}^{(\lambda)}) \geq 0$ imply the following GCB:

$$\Delta W_A \leq \left(1 - \frac{\beta_2}{\beta_1}\right) \Delta Q_{A,2} - \sum_{i=1}^2 \frac{\gamma_i}{\beta_1} \Delta Q_{B,i} \quad (3.6)$$

in response to the generalized heat $\Delta Q_{A,2}$ and $\Delta Q_{B,i}$, where we set $\beta_1 > 0$. In the following, we just focus on $\beta_1 > 0$ regime. When $\beta_1 < 0$ is true, the opposite inequality holds. As with the ordinary Carnot bound, this GCB is given only by generalized inverse temperatures. As mentioned in Remark 1.1, this bound does not include $\Delta Q_{A,1}$ since it is rather constrained if the other generalized heats are given.

The equality in (3.6) is achieved if and only if ΔS and $D(\rho'_{\text{Baths}} \| \tau_{\theta_0}^{(\lambda)})$ vanish simultaneously. In the thermodynamic limit with i.i.d. baths, an achievable protocol was shown for commutative quantities and non-commutative quantities [12]. However, this is possible only in the thermodynamic limit. When finite-size effects are taken into account, $D(\rho'_{\text{Baths}} \| \tau_{\theta_0}^{(\lambda)})$ cannot vanish. Hence, with finite size baths, GCB is never achieved. To derive a tight bound with finite-size effects, we have to consider how we can make $D(\rho'_{\text{Baths}} \| \tau_{\theta_0}^{(\lambda)})$ small under the scale λ as in [19]. We derive the fine-grained GCB in the next subsection.

3.3 Fine-grained generalized Carnot bound

We fix the generalized heat $\Delta Q_{A,2,\lambda}$ of Quantity A from Bath 2 and $\Delta Q_{B,i,\lambda}$ of quantity B from Bath i taking their scale dependence in account. We focus on the regime with

$$\Delta Q_{A,2,\lambda} = o(\lambda), \Delta Q_{B,i,\lambda} = o(\lambda) \quad (i = 1, 2). \quad (3.7)$$

These relations reflect the fact that the system $\mathcal{H}_{\text{Baths}}$ is used as just like baths in the sense that the ‘final inverse temperature’ converges to the initial one in thermodynamic limit, because the order of the generalized heats $\Delta Q_{A,2,\lambda}$, $\Delta Q_{B,i,\lambda}$ become smaller than the order $\mathcal{O}(\lambda)$ of $\frac{\partial \eta_{\lambda,2}}{\partial \beta_2}(\boldsymbol{\theta}_0)$ and $\frac{\partial \eta_{\lambda,i+2}}{\partial \gamma_i}(\boldsymbol{\theta}_0)$, which correspond to the respective ‘heat capacities’. Note that since the resultant state is not necessarily a generalized thermal state, the final inverse temperature is not necessarily well-defined. For a generic state ρ , we assign the ‘effective’ inverse temperature $\tilde{\boldsymbol{\theta}}_\lambda(\rho)$, which is defined as the generalized inverse temperature of the thermal state $\tau_{\tilde{\boldsymbol{\theta}}_\lambda(\rho)}^{(\lambda)}$ sharing the same expectation values:

$$\text{tr } A_{i,\lambda} \tau_{\tilde{\boldsymbol{\theta}}_\lambda(\rho)}^{(\lambda)} = \text{tr } A_{i,\lambda} \rho \quad (3.8)$$

$$\text{tr } B_{i,\lambda} \tau_{\tilde{\boldsymbol{\theta}}_\lambda(\rho)}^{(\lambda)} = \text{tr } B_{i,\lambda} \rho \quad (i = 1, 2). \quad (3.9)$$

Oppositely, if (3.7) does not hold, the generalized inverse temperatures of the baths change even in thermodynamic limit, so that GCB is not achievable. This is quite different from what the bath is in thermodynamics.

Then, the following fine-grained GCB holds:

Theorem 3.1 (Fine-grained generalized Carnot bound (FGCB)). *Let the generalized heats $\Delta Q_{A,2,\lambda}, \Delta Q_{B,1,\lambda}$ and $\Delta Q_{B,2,\lambda}$ satisfy (3.7). Then, we have*

$$\begin{aligned} \Delta W_A &\leq \left(1 - \frac{\beta_2}{\beta_1}\right) \Delta Q_{A,2,\lambda} - \sum_{i=1}^2 \frac{\gamma_i}{\beta_1} \Delta Q_{B,i,\lambda} \\ &\quad - C_{AA} \frac{\Delta Q_{A,2,\lambda}^2}{\lambda} - \sum_{i=1}^2 C_{AB}^i \frac{\Delta Q_{A,2,\lambda} \Delta Q_{B,i,\lambda}}{\lambda} - \sum_{i,j=1}^2 C_{BB}^{i,j} \frac{\Delta Q_{B,i,\lambda} \Delta Q_{B,j,\lambda}}{\lambda} + o\left(\frac{\|\mathbf{Q}_\lambda\|^2}{\lambda}\right) \\ &=: \Delta W_{A,\lambda}^{\text{opt}}(\mathbf{Q}_\lambda) + o\left(\frac{\|\mathbf{Q}_\lambda\|^2}{\lambda}\right), \end{aligned} \quad (3.10)$$

where we define $\mathbf{Q}_\lambda := (\Delta Q_{A,2,\lambda}, \Delta Q_{B,1,\lambda}, \Delta Q_{B,2,\lambda})$ and its norm $\|\mathbf{Q}_\lambda\|^2 := \beta_0^2 \Delta Q_{A,2,\lambda}^2 + \gamma_0^2 \Delta Q_{B,1,\lambda}^2 + \gamma_0^2 \Delta Q_{B,2,\lambda}^2$ with the unit generalized inverse temperatures β_0 and γ_0 to adjust the physical dimension, and the second order coefficients are given as follows:

$$C_{AA} = \frac{1}{2\beta_1} \left[g^{22}(\boldsymbol{\theta}_0) + \left(\frac{\beta_2}{\beta_1}\right)^2 g^{11}(\boldsymbol{\theta}_0) - 2\frac{\beta_2}{\beta_1} g^{12}(\boldsymbol{\theta}_0) \right], \quad (3.11)$$

$$C_{AB}^i = \frac{1}{\beta_1} \left[g^{2(i+2)}(\boldsymbol{\theta}_0) + \frac{\beta_2 \gamma_i}{\beta_1^2} g^{11}(\boldsymbol{\theta}_0) - \frac{\gamma_i}{\beta_1} g^{12}(\boldsymbol{\theta}_0) \right], \quad (3.12)$$

$$C_{BB}^{ij} = \frac{1}{2\beta_1} \left[g^{(i+2)(j+2)}(\boldsymbol{\theta}_0) + \frac{\gamma_i \gamma_j}{\beta_1^2} g^{11}(\boldsymbol{\theta}_0) - \frac{\gamma_j}{\beta_1} g^{1(i+2)}(\boldsymbol{\theta}_0) - \frac{\gamma_i}{\beta_1} g^{1(j+2)}(\boldsymbol{\theta}_0) \right], \quad (3.13)$$

where $(g^{ij}(\boldsymbol{\theta}_0))_{ij}$ is the inverse matrix of the asymptotic density of the canonical correlations $(g_{ij}(\boldsymbol{\theta}_0))_{ij}$ defined by (2.4), (2.8)².

The quantity $\Delta W_{A,\lambda}^{\text{opt}}(\mathbf{Q}_\lambda)$ gives an upper bound on the extraction of Quantity A including the finite-size effects of $\frac{\|\mathbf{Q}_\lambda\|^2}{\lambda}$ -order with the generalized heat \mathbf{Q}_λ . Note that ΔW_A may not be proper ‘work-like’ transfer of Quantity A , but rather possibly includes ‘heat-like’ transfer. Nevertheless, since any proper work-like transfer, namely $\Delta W'_A$, is included in the total transfer ΔW_A , we have $\Delta W'_A \leq \Delta W_A$. Thus, FGCB (3.10) is still true upper bound even for proper work-like extraction of Quantity A . The achievability of the bound is more delicate in this sense. In Sec. 4, including the battery system explicitly, we carefully construct an operation to achieve FGCB by avoiding hidden extra reservoir inside the battery.

The three terms of the second order $\frac{\|\mathbf{Q}_\lambda\|^2}{\lambda}$ in (3.10) express the finite-size effects, which are indeed always negative, so that FGCB does not exceed GCB. Remember that $g_{ij}(\boldsymbol{\theta}_0)$ is the asymptotic density of the Fisher information, and the elements of Fisher information are the canonical correlations of the baths’ quantities reflecting their non-commutativity. Thus, the second order terms reflect the effects of the fluctuation and correlation of the baths through $g^{ij}(\boldsymbol{\theta}_0)$. Therefore, the Fisher information, which is finer structure than just the temperatures of the baths is relevant in FGCB, differently from GCB (3.6) and the ordinary Carnot bound. Especially, correlations between the different baths are also taken into account. This result implies that we should consider the correlations of the conserved quantities of the baths to design better engine with finite-size baths.

Let us examine how to obtain better performance of generalized heat engines through interpreting the coefficients of the finite-size effect. FGCB is a direct consequence of the entropy increasing law due to the unitalness of the dynamics, as with GCB. As will be shown in the proof of Theorem 3.1 in later, for FGCB the second order term

$$-\frac{1}{2} \sum_{i,j=1}^4 g^{ij}(\boldsymbol{\theta}_0) \frac{\Delta X_{i,\lambda} \Delta X_{j,\lambda}}{\lambda} \quad (3.14)$$

in the entropy change is taken into account, where $\Delta X_{i,\lambda}$ is the variation in the expectation value of $X_{i,\lambda}$. The optimal performance is attained when the entropy change vanishes. Since this negative definite term (3.14) should be canceled for that, degradation of the optimal performance is caused. That is, the optimal performance approaches GCB as the baths get closer to the ideal baths in the sense that their state is unchanged through the operation. Conversely, variation of the state of the baths causes degradation of the optimal performance. In fact, the second order term (3.14) is expressed by the variation $\Delta\boldsymbol{\theta}$ in the inverse temperature as

$$\begin{aligned} & -\frac{1}{2} \sum_{i,j=1}^4 g^{ij}(\boldsymbol{\theta}_0) \frac{\Delta X_{i,\lambda} \Delta X_{j,\lambda}}{\lambda} \\ &= -\frac{1}{2} \sum_{i=1}^4 \Delta\theta^i \Delta X_{i,\lambda} + o\left(\frac{\Delta X_{i,\lambda} \Delta X_{j,\lambda}}{\lambda}\right) \end{aligned} \quad (3.15)$$

because

$$\Delta\theta^i = \sum_{j=1}^4 g^{ij}(\boldsymbol{\theta}_0) \frac{\Delta X_{j,\lambda}}{\lambda} + o\left(\frac{\Delta X_{j,\lambda}}{\lambda}\right). \quad (3.16)$$

²Physical dimension of (3.10) is consistent since each generalized inverse temperature has inverse dimension of its conjugate quantity.

Hence, the finite-size effect in FGCB reflects the linear response of the inverse temperature to the variation in $X_{j,\lambda}$ up to the order $\Delta X_{j,\lambda}/\lambda$. Indeed, the coefficients (3.11)-(3.13) are given in terms of the coefficient matrix $g^{ij}(\boldsymbol{\theta}_0)$. The coefficients (3.11)-(3.13) give the effect of the response of the inverse temperature on the optimal performance in a concrete form. From the above perspective, the smaller the response is, the better performance is achieved. Note that g^{ij} depends not only on the inverse temperature but also other parameters \mathbf{x} in general (see examples in Sec. 9) as $g^{ij}(\boldsymbol{\theta}; \mathbf{x})$. Especially, when $(g^{ij}(\boldsymbol{\theta}_0^{(1)}; \mathbf{x}_1))_{i,j} \leq (g^{ij}(\boldsymbol{\theta}_0^{(2)}; \mathbf{x}_2))_{i,j}$ holds as the matrix inequality, $(g^{ij}(\boldsymbol{\theta}_0^{(1)}; \mathbf{x}_1))_{i,j}$ gives better performance.

Proof of Theorem 3.1. The von Neumann entropy of the thermal states can be seen as a function of the expectation values by the following Legendre transformation:

$$S_\lambda(\boldsymbol{\eta}) := \min_{\tilde{\boldsymbol{\theta}}} \left[\sum_{i=1}^4 \tilde{\theta}^i \eta_i + \phi_\lambda(\tilde{\boldsymbol{\theta}}) \right]. \quad (3.17)$$

In this expression, S_λ is a function of the variable $\boldsymbol{\eta} = (\eta_1, \eta_2, \eta_3, \eta_4)$. For an inverse temperature $\boldsymbol{\theta}$, the function S_λ is actually related with the von Neumann entropy of the thermal state $\tau_{\boldsymbol{\theta}}^{(\lambda)}$ by the relation

$$S_\lambda(\boldsymbol{\eta}_\lambda(\boldsymbol{\theta})) = S(\tau_{\boldsymbol{\theta}}^{(\lambda)}), \quad (3.18)$$

where $\boldsymbol{\eta}_\lambda(\boldsymbol{\theta})$ is the dual coordinate of $\boldsymbol{\theta}$ composed of the expectation values defined by (2.3). In this sense, the variable $\boldsymbol{\eta}$ expresses the expectation values. If the final state ρ'_{Baths} of the baths satisfies $\Delta A_{i,\lambda} = \text{tr} A_{i,\lambda}(\rho'_{\text{Baths}} - \tau_{\boldsymbol{\theta}_0}^{(\lambda)}) = o(\lambda)$ and $\Delta B_{i,\lambda} = \text{tr} B_{i,\lambda}(\rho'_{\text{Baths}} - \tau_{\boldsymbol{\theta}_0}^{(\lambda)}) = o(\lambda)$, the effective inverse temperature $\boldsymbol{\theta}' := \tilde{\boldsymbol{\theta}}_\lambda(\rho'_{\text{Baths}})$ of ρ'_{Baths} exists for sufficiently large λ . That is, $\boldsymbol{\theta}'$ satisfies

$$\begin{aligned} \Delta \eta_{\lambda,i} &:= \eta_{\lambda,i}(\boldsymbol{\theta}') - \eta_{\lambda,i}(\boldsymbol{\theta}_0) = \Delta A_{i,\lambda}, \\ \Delta \eta_{\lambda,i+2} &:= \eta_{\lambda,i+2}(\boldsymbol{\theta}') - \eta_{\lambda,i+2}(\boldsymbol{\theta}_0) = \Delta B_{i,\lambda} \quad (i = 1, 2). \end{aligned} \quad (3.19)$$

Because the thermal state has the maximum entropy among the states with the same expectation values [12, 15, 17, 18]:

$$S(\tau_{\boldsymbol{\theta}}^{(\lambda)}) = \max_{\rho} \{S(\rho) | \tilde{\boldsymbol{\theta}}_\lambda(\rho) = \boldsymbol{\theta}\}, \quad (3.20)$$

the Taylor expansion of S_λ around $\boldsymbol{\eta}_\lambda(\boldsymbol{\theta}_0)$ yields

$$\begin{aligned} & S(\tau_{\boldsymbol{\theta}'}^{(\lambda)}) - S(\tau_{\boldsymbol{\theta}_0}^{(\lambda)}) \\ &= S_\lambda(\boldsymbol{\eta}_\lambda(\boldsymbol{\theta}')) - S_\lambda(\boldsymbol{\eta}_\lambda(\boldsymbol{\theta}_0)) \\ &= \sum_{i=1}^4 \theta_0^i \Delta \eta_{\lambda,i} - \frac{1}{2} \sum_{i,j=1}^4 J_\lambda^{ij}(\boldsymbol{\theta}_0) \Delta \eta_{\lambda,i} \Delta \eta_{\lambda,j} + \mathcal{O}\left(\frac{\|\Delta \boldsymbol{\eta}_\lambda\|^3}{\lambda^2}\right) \\ &= \sum_{i=1}^4 \theta_0^i \Delta \eta_{\lambda,i} - \frac{1}{2} \sum_{i,j=1}^4 g^{ij}(\boldsymbol{\theta}_0) \frac{\Delta \eta_{\lambda,i} \Delta \eta_{\lambda,j}}{\lambda} + o\left(\frac{\|\Delta \boldsymbol{\eta}_\lambda\|^2}{\lambda}\right) \\ &\geq S(\rho'_{\text{Baths}}) - S(\tau_{\boldsymbol{\theta}_0}^{(\lambda)}) \geq 0, \end{aligned} \quad (3.21)$$

where $J_\lambda^{ij}(\boldsymbol{\theta}_0)$ is the (i, j) -element of the inverse matrices of $(J_{\lambda,ij}(\boldsymbol{\theta}_0))$, and $\|\Delta \boldsymbol{\eta}_\lambda\| = \sqrt{\sum_{i=1}^4 (\Delta \eta_{\lambda,i})^2}$. The last inequality follows from the increasing of the entropy (3.4). We used the relation $\frac{\partial S_\lambda}{\partial \eta_i}(\boldsymbol{\eta}_\lambda(\boldsymbol{\theta})) = \theta^i$

to evaluate the coefficients of the Taylor expansion. We carried out the estimation of the third order derivatives based on Assumption 2.1 in the derivation of the order of the residual term in the second equality. The third equality follows from the estimation $J_\lambda^{ij}(\boldsymbol{\theta}_0) = \lambda^{-1}g^{ij}(\boldsymbol{\theta}_0) + o(\lambda^{-1})$, which holds uniformly on the neighborhood of the initial temperature. When $\Delta\eta_{\lambda,2} = \Delta A_{2,\lambda} = -\Delta Q_{A,2,\lambda}$, $\Delta\eta_{\lambda,i+2} = \Delta B_{i,\lambda} = -\Delta Q_{B,i,\lambda}$ ($i = 1, 2$) are given, by solving the equation $S_\lambda(\boldsymbol{\eta}_\lambda(\boldsymbol{\theta}')) - S_\lambda(\boldsymbol{\eta}_\lambda(\boldsymbol{\theta}_0)) = 0$ asymptotically with respect to $\Delta\eta_{\lambda,1}$, we obtain an upper bound for the possible value of $\Delta A_{1,\lambda} = \Delta\eta_{\lambda,1}$ as:

$$\begin{aligned} & -\beta_1\Delta A_{1,\lambda} \\ \leq & -\beta_2\Delta Q_{A,2,\lambda} - \sum_{i=1}^2 \gamma_i\Delta Q_{B,i,\lambda} \\ & -\beta_1 C_{AA} \frac{\Delta Q_{A,2,\lambda}^2}{\lambda} - \beta_1 \sum_{i=1}^2 C_{AB}^i \frac{\Delta Q_{A,2,\lambda}\Delta Q_{B,i,\lambda}}{\lambda} - \beta_1 \sum_{i,j=1}^2 C_{BB}^{i,j} \frac{\Delta Q_{B,i,\lambda}\Delta Q_{B,j,\lambda}}{\lambda} + o\left(\frac{\|\mathbf{Q}_\lambda\|^2}{\lambda}\right). \end{aligned} \quad (3.22)$$

Then, substituting (3.22) to $\Delta W_A = -\Delta A_{1,\lambda} + \Delta Q_{A,2,\lambda}$, we obtain (3.10). \square

We define the ideal final inverse temperature $\boldsymbol{\theta}_\lambda = (\beta_{\lambda 1}, \beta_{\lambda 2}, \gamma_{\lambda 1}, \gamma_{\lambda 2})$ associated with a vector \mathbf{Q}_λ of the generalized heat as

$$S(\tau_{\boldsymbol{\theta}_\lambda}^{(\lambda)}) = S(\tau_{\boldsymbol{\theta}_0}^{(\lambda)}) \quad (3.23)$$

$$\beta_{\lambda 1}\beta_1 \geq 0 \quad (3.24)$$

$$\text{tr } A_{2,\lambda}(\tau_{\boldsymbol{\theta}_0}^{(\lambda)} - \tau_{\boldsymbol{\theta}_\lambda}^{(\lambda)}) = \Delta Q_{A,2,\lambda} \quad (3.25)$$

$$\text{tr } B_{i,\lambda}(\tau_{\boldsymbol{\theta}_0}^{(\lambda)} - \tau_{\boldsymbol{\theta}_\lambda}^{(\lambda)}) = \Delta Q_{B,i,\lambda} \quad (i = 1, 2). \quad (3.26)$$

The equality in (3.10) is formally attained by the thermal state $\tau_{\boldsymbol{\theta}_\lambda}^{(\lambda)}$ at the ideal final inverse temperature $\boldsymbol{\theta}_\lambda = (\beta_{\lambda 1}, \beta_{\lambda 2}, \gamma_{\lambda 1}, \gamma_{\lambda 2})$ associated with \mathbf{Q}_λ . However, this state $\tau_{\boldsymbol{\theta}_\lambda}^{(\lambda)}$ is not necessarily achievable from $\tau_{\boldsymbol{\theta}_0}^{(\lambda)}$ by operations. In Sec. 4, for commutative observables, we show that FGCB is achievable in the asymptotic sense by constructing the operation which maps $\tau_{\boldsymbol{\theta}_0}^{(\lambda)}$ close to $\tau_{\boldsymbol{\theta}_\lambda}^{(\lambda)}$ instead of exactly to $\tau_{\boldsymbol{\theta}_\lambda}^{(\lambda)}$.

4 Achievability of FGCB by explicit construction of the protocol

In this section, we focus on the achievability of FGCB in ‘physical sense’. That is, as mentioned in Sec. 3.1, it is not enough to construct an implicit-battery operation to achieve the FGCB even though it satisfies the unitalness because the unitalness is only the necessary condition for the existence of an operation in the explicit-formulation that has no hidden heat-like transfer in the extracted amount.

To verify that our protocol achieves FGCB, we assume a stronger extensivity than Assumption 2.1.

Assumption 4.1. *The order of the deviation from the extensivity is sufficiently small so that there exists an $\alpha < \frac{1}{2}$ such that*

$$\phi_\lambda(\boldsymbol{\theta}) = \lambda\phi(\boldsymbol{\theta}) + \mathcal{O}(\lambda^\alpha), \quad (4.1)$$

$$\left(\frac{\partial}{\partial\theta^1}\right)^{l_1} \left(\frac{\partial}{\partial\theta^2}\right)^{l_2} \left(\frac{\partial}{\partial\theta^3}\right)^{l_3} \phi_\lambda(\boldsymbol{\theta}) = \left(\frac{\partial}{\partial\theta^1}\right)^{l_1} \left(\frac{\partial}{\partial\theta^2}\right)^{l_2} \left(\frac{\partial}{\partial\theta^3}\right)^{l_3} \lambda\phi(\boldsymbol{\theta}) + \mathcal{O}(\lambda^\alpha) \quad (4.2)$$

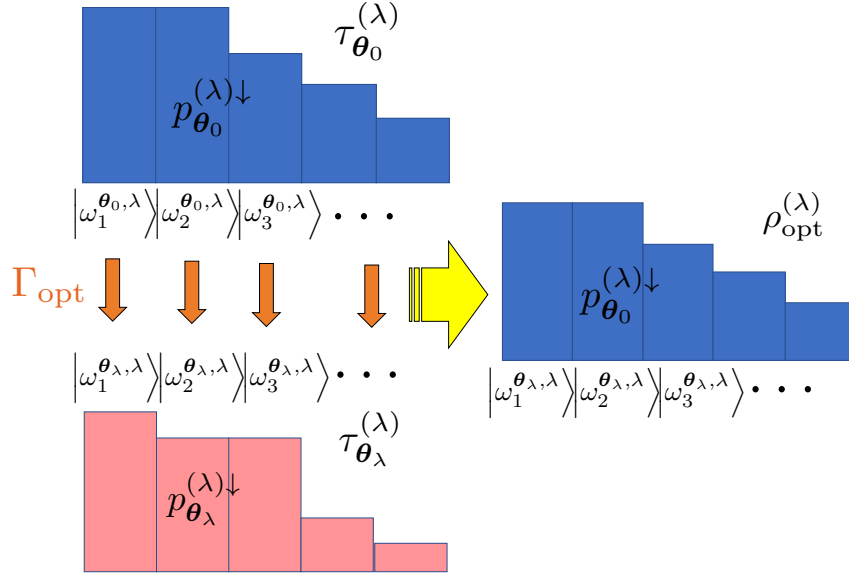


Figure 4.1: Schematic picture of the implicit operation Γ_{opt} . An ordering of the eigenstates $|\omega_1^{\theta_0, \lambda}\rangle, |\omega_2^{\theta_0, \lambda}\rangle, \dots$ is such that $|\omega_i^{\theta_0, \lambda}\rangle$ is mixed at the i -th largest probability $p_{\theta_0, \lambda}^{(\lambda)}(i)$ in the initial state $\tau_{\theta_0, \lambda}^{(\lambda)}$. Another ordering $|\omega_1^{\theta_\lambda, \lambda}\rangle, |\omega_2^{\theta_\lambda, \lambda}\rangle, \dots$ is such that $|\omega_i^{\theta_\lambda, \lambda}\rangle$ is mixed at the i -th largest probability $p_{\theta_\lambda}^{(\lambda)}(i)$ in the thermal state $\tau_{\theta_\lambda}^{(\lambda)}$ at the ideal final inverse temperature θ_λ . Γ_{opt} maps each $|\omega_i^{\theta_0, \lambda}\rangle$ to $|\omega_i^{\theta_\lambda, \lambda}\rangle$. In the resultant state $\rho_{\text{opt}}^{(\lambda)}$, $|\omega_i^{\theta_\lambda, \lambda}\rangle$ is mixed at the probability $p_{\theta_0}^{(\lambda)}(i)$ which was initially assigned to $|\omega_i^{\theta_0, \lambda}\rangle$.

hold instead of (2.5) and (2.6), where $0 < l_1 + l_2 + l_3 \leq 3$, $i_1, i_2, i_3 \in \{1, 2, 3, 4\}$. In addition, the matrix norms $\|A_{i, \lambda}\|, \|B_{i, \lambda}\|$ ($i = 1, 2$) are of order $\mathcal{O}(\lambda)$:

$$\|A_{i, \lambda}\| = \mathcal{O}(\lambda), \quad \|B_{i, \lambda}\| = \mathcal{O}(\lambda). \quad (4.3)$$

At first, we just focus on the commutative quantities in Sec. 4.1-4.4. We explicitly construct a protocol to achieve the equality in FGCB in the asymptotic sense up to $o\left(\frac{\|\mathbf{Q}_\lambda\|^2}{\lambda}\right)$ under the strict conservation law. The idea is to make the final state close to the thermal state with the ideal final inverse temperature θ_λ . Finally in Sec. 4.5, we extend the construction to the case of non-commutative quantities under the average conservation law.

4.1 Construction of the implicit-battery operation

To begin with, we construct an operation in the implicit-battery formulation to achieve the equality in FGCB for the case of commutative quantities. For this purpose, we choose the simultaneous eigenstates $|\omega\rangle$ to diagonalize $A_{1, \lambda}, A_{2, \lambda}, B_{1, \lambda}, B_{2, \lambda}$, so that the respective eigenvalues $a_{i, \lambda}(\omega)$ and $b_{i, \lambda}(\omega)$ ($i = 1, 2$) of $A_{i, \lambda}$ and $B_{i, \lambda}$ are labeled by ω . In our operation, we use the ordering of the simultaneous eigenstates $|\omega\rangle$ that depends on the inverse temperature coordinate θ and the scale λ . Given θ and λ , we diagonalize

$\tau_{\boldsymbol{\theta}}^{(\lambda)}$ as

$$\tau_{\boldsymbol{\theta}}^{(\lambda)} =: \sum_{i \in \mathbb{N}_{d_\lambda}} p_{\boldsymbol{\theta}}^{(\lambda)}(i) \left| \omega_i^{\boldsymbol{\theta}, \lambda} \right\rangle \left\langle \omega_i^{\boldsymbol{\theta}, \lambda} \right|, \quad (4.4)$$

where $\mathbb{N}_{d_\lambda} := \{1, 2, \dots, d_\lambda\}$. In the equation (4.4), we define the probability distribution $p_{\boldsymbol{\theta}}^{(\lambda)}$ composed of the eigenvalues of $\tau_{\boldsymbol{\theta}}^{(\lambda)}$ in descending order $p_{\boldsymbol{\theta}}^{(\lambda)}(1) \geq p_{\boldsymbol{\theta}}^{(\lambda)}(2) \geq \dots$, and accordingly label the simultaneous eigenstates $|\omega\rangle$ by defining the state $|\omega_i^{\boldsymbol{\theta}, \lambda}\rangle$. Although the ordering of the eigenstates is not unique because of the degeneracy, such multiplicity is totally irrelevant for our analysis. Thus, it is sufficient to arbitrarily choose an ordering for the eigenstates with the same eigenvalues. Given generalized heat amounts $\mathbf{Q}_\lambda = (\Delta Q_{A,2,\lambda}, \Delta Q_{B,1,\lambda}, \Delta Q_{B,2,\lambda})$, we have defined the ideal final inverse temperature $\boldsymbol{\theta}_\lambda$ by the conditions (3.23)-(3.26). Since the respective i -th largest eigenvalues $p_{\boldsymbol{\theta}_0}^{(\lambda)}(i)$ and $p_{\boldsymbol{\theta}_\lambda}^{(\lambda)}(i)$ of $\tau_{\boldsymbol{\theta}_0}^{(\lambda)}$ and $\tau_{\boldsymbol{\theta}_\lambda}^{(\lambda)}$ correspond to the different eigenstates from each other in general, the two states $|\omega_i^{\boldsymbol{\theta}_0, \lambda}\rangle$ and $|\omega_i^{\boldsymbol{\theta}_\lambda, \lambda}\rangle$ are different. Then, we consider a unital CPTP map on $\mathcal{H}_{\text{Baths}}$ which maps each eigenstate $|\omega_i^{\boldsymbol{\theta}_0, \lambda}\rangle$ to $|\omega_i^{\boldsymbol{\theta}_\lambda, \lambda}\rangle$. That is, we employ an operation $\Gamma_{\text{opt}}^{\mathbf{Q}_\lambda}$ to transform the initial state $\tau_{\boldsymbol{\theta}_0}^{(\lambda)}$ to the final state

$$\rho_{\text{opt}}^{(\lambda)} := \sum_i \left| \omega_i^{\boldsymbol{\theta}_\lambda, \lambda} \right\rangle \left\langle \omega_i^{\boldsymbol{\theta}_0, \lambda} \right| \tau_{\boldsymbol{\theta}_0}^{(\lambda)} \left| \omega_i^{\boldsymbol{\theta}_0, \lambda} \right\rangle \left\langle \omega_i^{\boldsymbol{\theta}_\lambda, \lambda} \right| = \sum_i p_{\boldsymbol{\theta}_0}^{(\lambda)}(i) \left| \omega_i^{\boldsymbol{\theta}_\lambda, \lambda} \right\rangle \left\langle \omega_i^{\boldsymbol{\theta}_\lambda, \lambda} \right|, \quad (4.5)$$

i.e.

$$\Gamma_{\text{opt}}^{\mathbf{Q}_\lambda}(\tau_{\boldsymbol{\theta}_0}^{(\lambda)}) = \rho_{\text{opt}}^{(\lambda)}. \quad (4.6)$$

In the final state $\rho_{\text{opt}}^{(\lambda)}$, the i -th largest probability $p_{\boldsymbol{\theta}_0}^{(\lambda)}(i)$ is assigned to the eigenstate $|\omega_i^{\boldsymbol{\theta}_\lambda, \lambda}\rangle$ instead of the original eigenstate $|\omega_i^{\boldsymbol{\theta}_0, \lambda}\rangle$. Since the operation $\Gamma_{\text{opt}}^{\mathbf{Q}_\lambda}$ exchanges the eigenstates, it satisfies the unital condition. Therefore, $\Gamma_{\text{opt}}^{\mathbf{Q}_\lambda} \otimes \text{id}_C$ is an implicit-battery operation on $\mathcal{H}_{\text{Baths}} \otimes \mathcal{H}_C$ and satisfies the unitalness. The cyclicity is also trivially satisfied. Especially, we do not use any catalytic effects of \mathcal{H}_C in this operation. Fig. 4.1 is a schematic picture of $\Gamma_{\text{opt}}^{\mathbf{Q}_\lambda}$.

In Sec. 4.4, we show that this final state $\rho_{\text{opt}}^{(\lambda)}$ achieves the FGCB. Although such a CPTP map $\Gamma_{\text{opt}}^{\mathbf{Q}_\lambda}$ is not unique, the proof of the achievability relies only on the final state $\rho_{\text{opt}}^{(\lambda)}$. However, since an implicit-battery operation is not necessarily extended to an explicit-battery operation, before showing the achievability of FGCB, we have to construct an explicit-battery unitary operation to be reduced to a CPTP map

$\Gamma_{\text{opt}}^{\mathbf{Q}_\lambda}$ satisfying (4.6). Then, under an explicit battery given in Sec. 4.2, we construct such a unitary operation in Sec. 4.3.

4.2 Explicit battery

To show the tightness of FGCB, we should construct a unitary operation on the whole system in the appropriate 'explicit' formulation as mentioned in Sec. 3.1. To do so, we fix an explicit formulation by choosing an appropriate battery system \mathcal{H}_W and reasonable constraints on the operations with explicit batteries as follows.

As in [12], we assume that the battery system \mathcal{H}_W is $\mathcal{H}_{W_a} \otimes \mathcal{H}_{W_b} = L^2(\mathbb{R})^{\otimes 2}$, where the components $\mathcal{H}_{W_a} = L^2(\mathbb{R})$ and $\mathcal{H}_{W_b} = L^2(\mathbb{R})$ of the tensor product correspond to the degree of freedom for Quantities A and B , respectively. Let the respective battery observables A_W and B_W of Quantities A and B be given as $A_W = c_a \hat{x}_a$, $B_W = c_b \hat{x}_b$, where c_a and c_b are the constants, \hat{x}_a and \hat{x}_b are the independent position operators. We can also construct the battery system with discrete spectrum in the same way as [31, 35]. Note that such a bit unphysical doubly infinite spectrum of the battery is an idealization to focus on the theoretical limit to the performance of the engine, which is similar to that we do not care about the length of the string suspending the weight in thermodynamics.

To show that the FGCB is really achieved by properly work-like transportation of the quantity, it is not enough to just impose the conditions A1, A2 on the operations on $\mathcal{H}_{\text{Baths}} \otimes \mathcal{H}_C$ under which FGCB is verified. Stronger conditions are needed on the dynamics of the whole system $\mathcal{H}_{\text{Baths}} \otimes \mathcal{H}_C \otimes \mathcal{H}_W$ with the explicit battery \mathcal{H}_W fixed above. As reasonable constraints for our explicit-battery formulation, we consider the following conditions B1-B4 on a unitary operation U on $\mathcal{H}_{\text{Baths}} \otimes \mathcal{H}_C \otimes \mathcal{H}_W$ to be allowed as a dynamics of the generalized heat engine. In other words, if a unitary U satisfies the following conditions B1-B4, there exists a generalized heat engine to implement U per unit cycle whose output work is

$$\Delta W_A = \text{tr } A_W U \rho_0 U^\dagger - \text{tr } A_W \rho_0 \quad (4.7)$$

for the initial state $\rho_0 = \tau_{\theta_0}^{(\lambda)} \otimes \rho_C \otimes \rho_W$ of the total system. In fact, as we mention in the last paragraph of this subsection, such an allowed operation U reduces to an operation on $\mathcal{H}_{\text{Baths}} \otimes \mathcal{H}_C$ satisfying the constraints A1, A2 on the implicit-battery operation (Definition 3.1).

B1. Strict conservation law:

$$\left[\sum_{j=1}^2 A_{j,\lambda} + A_W, U \right] = \left[\sum_{j=1}^2 B_{j,\lambda} + B_W, U \right] = 0. \quad (4.8)$$

B2. Cyclicity of the engine:

There exists a state ρ_C of \mathcal{H}_C such that

$$\text{tr}_{\mathcal{H}_{\text{Baths}} \otimes \mathcal{H}_W} U(\tau_{\theta_0}^{(\lambda)} \otimes \rho_C \otimes \rho_W) U^\dagger = \rho_C \quad (4.9)$$

holds for an arbitrary initial state ρ_W of the battery.

B3. Independence of the initial state of the battery ('no-cheating condition 1'):

$$\text{tr}_{\mathcal{H}_W} U(\tau_{\theta_0}^{(\lambda)} \otimes \rho_C \otimes \rho_{W,1}) U^\dagger = \text{tr}_{\mathcal{H}_W} U(\tau_{\theta_0}^{(\lambda)} \otimes \rho_C \otimes \rho_{W,2}) U^\dagger \quad (4.10)$$

for any states $\rho_{W,1}, \rho_{W,2}$ of \mathcal{H}_W .

B4. Translational symmetry ('no-cheating condition 2'):

$$[\Delta_A^\epsilon, U] = [\Delta_B^\epsilon, U] = 0, \quad (4.11)$$

where we define the translation operators of A_W as

$$\Delta_A^\epsilon := \exp(-i\epsilon \hat{p}_a) \quad (4.12)$$

by the momentum operator \hat{p}_a conjugate to \hat{x}_a . The translation operator Δ_B^ϵ of B_W is similarly defined.

Unitarity is required to prohibit using any resource outside of $\mathcal{H}_{\text{Baths}} \otimes \mathcal{H}_C \otimes \mathcal{H}_W$. In addition to the conservation laws and cyclicity of the engine, we demand the no-cheating condition as in [12, 32, 39]. Independence of the initial state of the battery (Condition B3) is to prevent ourselves from cheatingly using the battery as other than a battery, e.g. as like a ‘cold reservoir’. That is, we guarantee that there is no hidden heat-like transfer of each quantity with the battery itself, which is non-trivial to verify in quantum thermodynamics. Indeed, if there is such a heat-like transfer, it must depend on the state of the battery. As Condition B4, translational symmetry is individually imposed since it is not shown to automatically follow from Condition B3, and vice versa. Indeed, the translational symmetry of the battery is needed because it guarantees that the generalized heat engine works properly even when we cannot control the initial state on the battery and can observe only the translation of the battery [32]. The relevance of this requirement can be found by considering the typical case where the battery is given as the ‘height’ of the weight. Such extreme symmetries of the battery are sufficient to remove undesired effects from the battery.

Furthermore, the reduced dynamics $\Gamma(\tau_{\theta_0}^{(\lambda)} \otimes \rho_C) = \text{tr}_{\mathcal{H}_W} U(\tau_{\theta_0}^{(\lambda)} \otimes \rho_C \otimes \rho_W)U^\dagger$ on $\mathcal{H}_{\text{Baths}} \otimes \mathcal{H}_C$ is unital for arbitrary ρ_W [12, 32]. Thus, an operation in this explicit-battery formulation indeed reduces to an implicit-battery operation defined in Definition 3.1. Hence, for showing the achievability of FGCB, it is enough to construct an operation to achieve it under these constraints. In the next subsection, we construct a global unitary operation to achieve FGCB under these conditions.

4.3 Construction of the ‘explicit’ operation

Now, we construct a global unitary operation which is reduced to an operation $\Gamma_{\text{opt}}^{\mathbf{Q}_\lambda}$ satisfying (4.6). Using the translation operators Δ_A^ϵ , Δ_B^ϵ , and the state $|\omega_i^{\theta_i, \lambda}\rangle$ defined in (4.12), and (4.4) respectively, we define the unitary operator $U_{\text{opt}}^{(\lambda)}(\mathbf{Q}_\lambda)$ on $\mathcal{H}_{\text{Baths}} \otimes \mathcal{H}_W$ depending on $\mathbf{Q}_\lambda = (\Delta Q_{A,2,\lambda}, \Delta Q_{B,1,\lambda}, \Delta Q_{B,2,\lambda})$ as follows:

$$\begin{aligned}
& U_{\text{opt}}^{(\lambda)}(\mathbf{Q}_\lambda) \\
& := \sum_i \left| \omega_i^{\theta_i, \lambda} \right\rangle \left\langle \omega_i^{\theta_0, \lambda} \right| \\
& \quad \otimes \Delta_A^{c_a^{-1}(a_{1,\lambda}(\omega_i^{\theta_0, \lambda}) + a_{2,\lambda}(\omega_i^{\theta_0, \lambda}) - a_{1,\lambda}(\omega_i^{\theta_i, \lambda}) - a_{2,\lambda}(\omega_i^{\theta_i, \lambda}))} \otimes \Delta_B^{c_b^{-1}(b_{1,\lambda}(\omega_i^{\theta_0, \lambda}) + b_{2,\lambda}(\omega_i^{\theta_0, \lambda}) - b_{1,\lambda}(\omega_i^{\theta_i, \lambda}) - b_{2,\lambda}(\omega_i^{\theta_i, \lambda}))}.
\end{aligned} \tag{4.13}$$

Note that \mathbf{Q}_λ does not have the meaning of generalized heat at this moment. That is, the amount of the generalized heat of this protocol $U_{\text{opt}}^{(\lambda)}(\mathbf{Q}_\lambda)$ has not guaranteed to be \mathbf{Q}_λ . Instead, \mathbf{Q}_λ should be regarded just as a variable, though it will turn out that it indeed asymptotically corresponds to the generalized heat of this protocol.

For an arbitrary fixed initial state ρ_W of the battery, we define the reduced dynamics $\Gamma_{\text{opt}}^{\mathbf{Q}_\lambda}$ as an implicit-battery protocol by $\Gamma_{\text{opt}}^{\mathbf{Q}_\lambda}(\rho) = \text{tr}_{\mathcal{H}_W} U_{\text{opt}}^{(\lambda)}(\mathbf{Q}_\lambda)(\rho \otimes \rho_W)U_{\text{opt}}^{(\lambda)}(\mathbf{Q}_\lambda)^\dagger$. The condition $\Gamma_{\text{opt}}^{\mathbf{Q}_\lambda}(\tau_{\theta_0}^{(\lambda)}) = \rho_{\text{opt}}^{(\lambda)}$ is satisfied regardless of the state ρ_W . Thus, once the unitary operator $U_{\text{opt}}^{(\lambda)}(\mathbf{Q}_\lambda)$ satisfies the conditions (4.8)-(4.11), we find that the reduced dynamics $\Gamma_{\text{opt}}^{\mathbf{Q}_\lambda}$ is the desired implicit-battery operation satisfying the property given in Sec. 4.1.

In fact, the unitary operator $U_{\text{opt}}^{(\lambda)}(\mathbf{Q}_\lambda)$ satisfies the strict conservation laws (4.8) since the battery part of the operation absorbs the transition of the corresponding quantity of the baths. No-cheating condition (4.10), (4.11) is also easily verified. The global unitary operation on $\mathcal{H}_{\text{Baths}} \otimes \mathcal{H}_W \otimes \mathcal{H}_C$ is $U_{\text{opt}}^{(\lambda)}(\mathbf{Q}_\lambda) \otimes I_C$,

which obviously satisfies the cyclicity (4.9). Therefore, this global unitary operation satisfies all the conditions of the explicit formulation. Thus, the final state $\rho_{\text{opt}}^{(\lambda)}$ is verified to be attained by an allowed operation.

In the next subsection, we show that this final state $\rho_{\text{opt}}^{(\lambda)}$ really achieves the equality in FGCB in the asymptotic sense.

4.4 Achievement of the equality in FGCB

Our goal is to show that our constructed protocol $U_{\text{opt}}^{(\lambda)}(\mathbf{Q}_\lambda) \otimes I_C$ achieves the maximum extraction $\Delta W_{A,\lambda}^{\text{opt}}(\mathbf{Q}_\lambda)$ except for $o\left(\frac{\|\mathbf{Q}_\lambda\|^2}{\lambda}\right)$ order of error terms. The work output ΔW_A of a generalized heat engine implementing an allowed unitary operation U is defined by (4.7) with the initial state $\rho_0 = \tau_{\theta_0}^{(\lambda)} \otimes \rho_C \otimes \rho_W$. The strict conservation law B1 of Quantity A implies the conservation of the sum of the average values of them:

$$\text{tr}(A_{1,\lambda} + A_{2,\lambda} + A_W)U\rho_0U^\dagger = \text{tr}(A_{1,\lambda} + A_{2,\lambda} + A_W)\rho_0. \quad (4.14)$$

Hence, if the final state of the baths is ρ'_{Baths} , the work output is given by

$$\Delta W_A = \text{tr}(A_{1,\lambda} + A_{2,\lambda})(\tau_{\theta_0}^{(\lambda)} - \rho'_{\text{Baths}}). \quad (4.15)$$

Then, our goal is to show the following theorem as the achievement of FGCB by the protocol we have constructed. We denote that $f(\lambda)/g(\lambda) \rightarrow 0$ ($\lambda \rightarrow \infty$) by $f(\lambda) \ll g(\lambda)$.

Theorem 4.1. *Let $A_{i,\lambda}$ and $B_{i,\lambda}$ ($i = 1, 2$) be mutually commutative. We assume that Assumption 4.1 is satisfied. For any $\mathbf{Q}_\lambda = (\Delta Q_{A,2,\lambda}, \Delta Q_{B,1,\lambda}, \Delta Q_{B,2,\lambda})$, there exists a generalized heat engine implementing $U_{\text{opt}}^{(\lambda)}(\mathbf{Q}_\lambda) \otimes I_C$ in the sense of the explicit-battery formulation B1-B4. Especially, the final state $\rho_{\text{opt}}^{(\lambda)} = \text{tr}_{\mathcal{H}_W} U_{\text{opt}}^{(\lambda)}(\mathbf{Q}_\lambda)(\tau_{\theta_0}^{(\lambda)} \otimes \rho_W)U_{\text{opt}}^{(\lambda)}(\mathbf{Q}_\lambda)^\dagger$ of the baths is independent of the initial state of the battery ρ_W . If \mathbf{Q}_λ satisfies*

$$\lambda^{\frac{5}{8}} \ll \|\mathbf{Q}_\lambda\| \ll \lambda, \quad (4.16)$$

then the final state $\rho_{\text{opt}}^{(\lambda)}$ of the baths satisfies

$$\text{tr} A_{i,\lambda}\rho_{\text{opt}}^{(\lambda)} = \text{tr} A_{i,\lambda}\tau_{\theta_\lambda}^{(\lambda)} + o\left(\frac{\|\mathbf{Q}_\lambda\|^2}{\lambda}\right) \quad (4.17)$$

$$\text{tr} B_{i,\lambda}\rho_{\text{opt}}^{(\lambda)} = \text{tr} B_{i,\lambda}\tau_{\theta_\lambda}^{(\lambda)} + o\left(\frac{\|\mathbf{Q}_\lambda\|^2}{\lambda}\right) \quad (i = 1, 2). \quad (4.18)$$

Because $\tau_{\theta_\lambda}^{(\lambda)}$ attains FGCB with the generalized heat \mathbf{Q}_λ , it immediately follows from Theorem 4.1 that we can extract the maximum amount $\Delta W_{A,\lambda}^{\text{opt}}(\mathbf{Q}_\lambda)$ of the work given in FGCB (3.10) in the asymptotic sense up to $o\left(\frac{\|\mathbf{Q}_\lambda\|^2}{\lambda}\right)$ if we run the protocol $U_{\text{opt}}^{(\lambda)}(\mathbf{Q}_\lambda) \otimes I_C$ with appropriate order of \mathbf{Q}_λ . Though the actual generalized heat of this protocol has the error up to $o\left(\frac{\|\mathbf{Q}_\lambda\|^2}{\lambda}\right)$,

$$\Delta W_{A,\lambda}^{\text{opt}}\left(\mathbf{Q}_\lambda + o\left(\frac{\|\mathbf{Q}_\lambda\|^2}{\lambda}\right)\right) = \Delta W_{A,\lambda}^{\text{opt}}(\mathbf{Q}_\lambda) \quad (4.19)$$

is obvious from FGCB. Thus, the equality in FGCB is achieved by our protocol asymptotically up to $o\left(\frac{\|\mathbf{Q}_\lambda\|^2}{\lambda}\right)$, hence FGCB is tight. In other words, we have the following corollary.

Corollary 4.1. *Let $A_{i,\lambda}$ and $B_{i,\lambda}$ ($i = 1, 2$) be mutually commutative. Under Assumption 4.1 and (4.16), the generalized heat of the heat engine implementing the operation $U_{\text{opt}}^{(\lambda)}(\mathbf{Q}_\lambda) \otimes I_C$ coincides with \mathbf{Q}_λ up to $o\left(\frac{\|\mathbf{Q}_\lambda\|^2}{\lambda}\right)$ as follows:*

$$\text{tr } A_{2,\lambda}(\tau_{\theta_0}^{(\lambda)} - \rho_{\text{opt}}^{(\lambda)}) = \Delta Q_{A,2,\lambda} + o\left(\frac{\|\mathbf{Q}_\lambda\|^2}{\lambda}\right) \quad (4.20)$$

$$\text{tr } B_{i,\lambda}(\tau_{\theta_0}^{(\lambda)} - \rho_{\text{opt}}^{(\lambda)}) = \Delta Q_{B,i,\lambda} + o\left(\frac{\|\mathbf{Q}_\lambda\|^2}{\lambda}\right) \quad (i = 1, 2). \quad (4.21)$$

Up to $o\left(\frac{\|\mathbf{Q}_\lambda\|^2}{\lambda}\right)$, the work output of Quantity A of this engine equals to the maximum work with the generalized heat \mathbf{Q}_λ as follows:

$$\Delta W_A = \text{tr}(A_{1,\lambda} + A_{2,\lambda})(\tau_{\theta_0}^{(\lambda)} - \rho_{\text{opt}}^{(\lambda)}) = \Delta W_{A,\lambda}^{\text{opt}}(\mathbf{Q}_\lambda) + o\left(\frac{\|\mathbf{Q}_\lambda\|^2}{\lambda}\right). \quad (4.22)$$

Hence, FGCB is asymptotically achieved up to $o\left(\frac{\|\mathbf{Q}_\lambda\|^2}{\lambda}\right)$ by this engine.

We remark that the final state $\rho_{\text{opt}}^{(\lambda)}$ is not uniquely determined because it depends on the choices of the orderings of states $\left\{|\omega_i^{\theta_0,\lambda}\rangle\right\}_i, \left\{|\omega_i^{\theta_\lambda,\lambda}\rangle\right\}_i$ among their multiplicity because of the degeneracy. However, any final state $\rho_{\text{opt}}^{(\lambda)}$ satisfies Theorem 4.1 because any choice makes no difference in the following analysis.

Furthermore, since the dynamics on \mathcal{H}_C is simply the identity in our protocol, we do not use catalytic effects at all. This construction shows that catalytic effects work in small order of $o\left(\frac{\|\mathbf{Q}_\lambda\|^2}{\lambda}\right)$ for the optimal performance. Of course, since our protocol achieves GCB in thermodynamic limit, our protocol with the generic scaling λ is novel even for the regime of thermodynamic limit. Although our derivation imposed the condition on the norm of the observables for the technical simplicity, there is possibility to remove it. The conditions (4.1) and (4.2) with $\alpha < \frac{1}{2}$ are also needed for our analysis to work, which seem to be more essential. The reason is that larger order than λ^α ($\alpha \geq \frac{1}{2}$) of the deviation from the extensivity (2.5), (2.6) possibly degrades the performance of the engine.

The idea of the proof of Theorem 4.1 is as follows. The ideal thermal state $\tau_{\theta_\lambda}^{(\lambda)}$ attains the equality in FGCB (3.10) under the given heat amounts (3.25) and (3.26) by its definition, though this state itself is not necessarily achieved from the initial state $\tau_{\theta_0}^{(\lambda)}$ through an allowed operation. Thus, in order to prove Theorem 4.1, it is sufficient to show that each expectation value of $\rho_{\text{opt}}^{(\lambda)}$ is close to that of $\tau_{\theta_\lambda}^{(\lambda)}$ in the order of $o\left(\frac{\|\mathbf{Q}_\lambda\|^2}{\lambda}\right)$. Then, we firstly observe the relation between the differences $|\text{tr } A_{i,\lambda}(\tau_{\theta_\lambda}^{(\lambda)} - \rho_{\text{opt}}^{(\lambda)})|$, $|\text{tr } B_{i,\lambda}(\tau_{\theta_\lambda}^{(\lambda)} - \rho_{\text{opt}}^{(\lambda)})|$ in the expectation values and the relative entropy $D(\rho_{\text{opt}}^{(\lambda)}\|\tau_{\theta_\lambda}^{(\lambda)})$. To do so, it is sufficient to focus on the thermal state at the effective inverse temperature $\xi_\lambda := \tilde{\theta}_\lambda(\rho_{\text{opt}}^{(\lambda)})$ of $\rho_{\text{opt}}^{(\lambda)}$ since it shares the expectation values with $\rho_{\text{opt}}^{(\lambda)}$ as

$$\eta_{\lambda,i}(\xi_\lambda) = \text{tr } A_{i,\lambda}\rho_{\text{opt}}^{(\lambda)}, \quad (4.23)$$

$$\eta_{\lambda,i+2}(\xi_\lambda) = \text{tr } B_{i,\lambda}\rho_{\text{opt}}^{(\lambda)} \quad (i = 1, 2). \quad (4.24)$$

Any full-rank state always has its effective inverse temperature. In fact, $\rho_{\text{opt}}^{(\lambda)}$ has full rank by definition. Then, we show the following lemma.

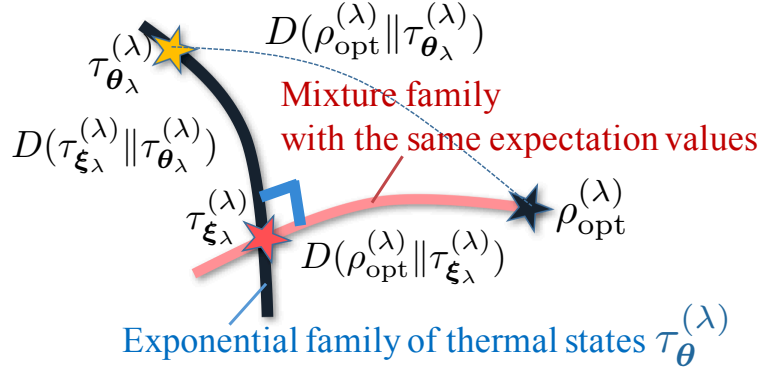


Figure 4.2: Information geometric positional relationships for the Pythagorean theorem. The states sharing the same expectation values form a mixture family. The family of the thermal states parametrized by inverse temperatures is an exponential family. The definition and details of the exponential and the mixture families of the states are given in Appendix A.

Lemma 4.1. *For the effective inverse temperature ξ_{λ} of $\rho_{\text{opt}}^{(\lambda)}$, we have*

$$2D(\rho_{\text{opt}}^{(\lambda)} \parallel \tau_{\theta_{\lambda}}^{(\lambda)}) \max_{t \in [0,1]} \|(J_{\lambda,ij}(\mathbf{s}_{\lambda}(t)))_{ij}\| \geq \|\boldsymbol{\eta}_{\lambda}(\boldsymbol{\theta}_{\lambda}) - \boldsymbol{\eta}_{\lambda}(\boldsymbol{\xi}_{\lambda})\|^2, \quad (4.25)$$

where we denote the matrix whose (i, j) -component is a_{ij} by $(a_{ij})_{ij}$, and $\mathbf{s}_{\lambda}(t)$ is the inverse temperature to satisfy $\boldsymbol{\eta}_{\lambda}(\mathbf{s}_{\lambda}(t)) = t\boldsymbol{\eta}_{\lambda}(\boldsymbol{\theta}_{\lambda}) + (1-t)\boldsymbol{\eta}_{\lambda}(\boldsymbol{\xi}_{\lambda})$. Here, $\|A\|$ for a matrix A is the matrix norm.

Proof. To verify Lemma 4.1, we focus on the following information geometric estimations. In fact, since $\rho_{\text{opt}}^{(\lambda)}$ has full rank, we can apply the methods of information geometry in Appendix A. Since ξ_{λ} is the effective inverse temperature of $\rho_{\text{opt}}^{(\lambda)}$, $\tau_{\xi_{\lambda}}^{(\lambda)}$ is the thermal state sharing the expectation values of $A_{i,\lambda}$ and $B_{i,\lambda}$ with $\rho_{\text{opt}}^{(\lambda)}$. Thus, applying the Pythagorean theorem (Lemma A.3 in Appendix A.2), we obtain

$$D(\rho_{\text{opt}}^{(\lambda)} \parallel \tau_{\theta_{\lambda}}^{(\lambda)}) = D(\rho_{\text{opt}}^{(\lambda)} \parallel \tau_{\xi_{\lambda}}^{(\lambda)}) + D(\tau_{\xi_{\lambda}}^{(\lambda)} \parallel \tau_{\theta_{\lambda}}^{(\lambda)}) \geq D(\tau_{\xi_{\lambda}}^{(\lambda)} \parallel \tau_{\theta_{\lambda}}^{(\lambda)}) \quad (4.26)$$

as illustrated in Fig. 4.2. Furthermore, applying the relation (A.14) in Appendix A.2, we have the following relation between the relative entropy and expectation values:

$$\begin{aligned} & D(\tau_{\xi_{\lambda}}^{(\lambda)} \parallel \tau_{\theta_{\lambda}}^{(\lambda)}) \\ &= \int_0^1 \sum_{ij} (\eta_{\lambda,i}(\boldsymbol{\theta}_{\lambda}) - \eta_{\lambda,i}(\boldsymbol{\xi}_{\lambda})) (\eta_{\lambda,j}(\boldsymbol{\theta}_{\lambda}) - \eta_{\lambda,j}(\boldsymbol{\xi}_{\lambda})) J_{\lambda}^{ij}(\mathbf{s}_{\lambda}(t)) t dt \\ &\geq \frac{1}{2} \|\boldsymbol{\eta}_{\lambda}(\boldsymbol{\theta}_{\lambda}) - \boldsymbol{\eta}_{\lambda}(\boldsymbol{\xi}_{\lambda})\|^2 \min_{t \in [0,1]} \frac{1}{\|(J_{\lambda,ij}(\mathbf{s}_{\lambda}(t)))_{ij}\|}, \end{aligned} \quad (4.27)$$

where we used the fact that the maximum eigenvalue of $(J_{\lambda,ij}(\mathbf{s}_{\lambda}(t)))_{ij}$ is equal to $\|(J_{\lambda,ij}(\mathbf{s}_{\lambda}(t)))_{ij}\|$ since $(J_{\lambda,ij}(\mathbf{s}_{\lambda}(t)))_{ij}$ is a positive matrix. Combining (4.27) with (4.26), we obtain (4.25). \square

By Lemma 4.1, our problem is reduced to the estimation of the relative entropy $D(\rho_{\text{opt}}^{(\lambda)} \parallel \tau_{\theta_{\lambda}}^{(\lambda)})$ and Fisher information $\|(J_{\lambda,ij}(\mathbf{s}_{\lambda}(t)))_{ij}\|$ on the left hand side (LHS) of (4.25) because the difference in the expectation value of each quantity between $\tau_{\theta_{\lambda}}^{(\lambda)}$ and $\rho_{\text{opt}}^{(\lambda)}$ are smaller than $\|\boldsymbol{\eta}_{\lambda}(\boldsymbol{\theta}_{\lambda}) - \boldsymbol{\eta}_{\lambda}(\boldsymbol{\xi}_{\lambda})\|$. Sec. 5-7 are devoted to the estimation of them. After that, we prove Theorem 4.1 in Sec. 8.

4.5 Non-commutative quantities

We extend our protocol to the case where $A_{i,\lambda}$ and $B_{j,\lambda}$ are not commutative. We use the same battery system $\mathcal{H}_W = \mathcal{H}_{W_a} \otimes \mathcal{H}_{W_b}$. Especially, we still assume that the battery observables A_W and B_W commute. This is natural since it is sufficient to use an individual system for each quantity. In this case, instead of the strict conservation law (4.8), we just impose the average conservation law:

B1*. Average conservation law:

$$\text{tr} U(\tau_{\theta_0}^{(\lambda)} \otimes \rho_C \otimes \rho_W) U^\dagger \left(\sum_{j=1}^2 A_{j,\lambda} + A_W \right) = \text{tr} \left(\tau_{\theta_0}^{(\lambda)} \otimes \rho_C \otimes \rho_W \right) \left(\sum_{j=1}^2 A_{j,\lambda} + A_W \right), \quad (4.28)$$

$$\text{tr} U(\tau_{\theta_0}^{(\lambda)} \otimes \rho_C \otimes \rho_W) U^\dagger \left(\sum_{j=1}^2 B_{j,\lambda} + B_W \right) = \text{tr} \left(\tau_{\theta_0}^{(\lambda)} \otimes \rho_C \otimes \rho_W \right) \left(\sum_{j=1}^2 B_{j,\lambda} + B_W \right). \quad (4.29)$$

The other constraints B2-B4 are the same as the commutative case. That is, we consider the conditions B1*, B2-B4 on a unitary operation U on $\mathcal{H}_{\text{Baths}} \otimes \mathcal{H}_C \otimes \mathcal{H}_W$ to be allowed as a dynamics of the generalized heat engine.

As for the first law of the thermodynamics, Lostaglio *et al.* [34] pointed out that some external resource of the coherence may be missed in the formulation without the strict conservation of the energy. That is, the coherence with respect to the energy eigenstates can be increased by an operation with just the average conservation, though it is impossible for strictly energy conservative operations. This implies that some resource of the coherence is implicitly used to implement such an operation. This may be the case also for generic multiple conservative quantities under the consideration. Thus, it may be appropriate to call it ‘semi-explicit’ battery formulation, reflecting the possibility of the lack of some resource in the formulation, while the battery system is explicitly taken into account³. We show the achievability for non-commutative quantities in this semi-explicit battery formulation in the following.

We construct a global unitary operation satisfying B1*, B2-B4. Because of non-commutativity, the simultaneous eigenbasis no longer exists. However, $\tau_{\theta}^{(\lambda)}$ is diagonalized by a basis depending on θ and λ . Thus, for a given vector \mathbf{Q}_λ , we denote the diagonalization of $\tau_{\theta_0}^{(\lambda)}$ and $\tau_{\theta_\lambda}^{(\lambda)}$ respectively by:

$$\tau_{\theta_0}^{(\lambda)} = \sum_{i \in \mathbb{N}_{d_\lambda}} p_{\theta_0}^{(\lambda)}(i) |\psi_i\rangle\langle\psi_i| \quad (4.30)$$

$$\tau_{\theta_\lambda}^{(\lambda)} = \sum_{i \in \mathbb{N}_{d_\lambda}} p_{\theta_\lambda}^{(\lambda)}(i) |\varphi_i\rangle\langle\varphi_i|, \quad (4.31)$$

where $p_{\theta_0}^{(\lambda)}(1) \geq p_{\theta_0}^{(\lambda)}(2) \geq \dots$ and $p_{\theta_\lambda}^{(\lambda)}(1) \geq p_{\theta_\lambda}^{(\lambda)}(2) \geq \dots$ hold. Note that $|\psi_i\rangle, |\varphi_i\rangle$ depend also on λ , though we omit the notation for simplicity. Then, we define $\rho_{\text{opt,nc}}^{(\lambda)} := \sum_i |\varphi_i\rangle\langle\psi_i| \tau_{\theta_0}^{(\lambda)} |\psi_i\rangle\langle\varphi_i|$ as with the commutative case.

³However, as for the energy conservation, [34] also pointed out that if some resource of coherence is appropriately considered through the method by [35], the results under the average conservation would be revived under the strict conservation law. This is also possibly the case for the multiple conservative quantities.

Then, we construct the protocol in the explicit-battery formulation. With the same battery system as the commutative case, we define the unitary operator $U_{\text{opt,nc}}^{(\lambda)}(\mathbf{Q}_\lambda)$ on $\mathcal{H}_{\text{Baths}} \otimes \mathcal{H}_W$ as

$$U_{\text{opt,nc}}^{(\lambda)}(\mathbf{Q}_\lambda) := \sum_i |\varphi_i\rangle\langle\psi_i| \otimes \Delta_A^{c_a^{-1}(\langle\psi_i|\sum_{i=1}^2 A_{i,\lambda}|\psi_i\rangle - \langle\varphi_i|\sum_{i=1}^2 A_{i,\lambda}|\varphi_i\rangle)} \otimes \Delta_B^{c_b^{-1}(\langle\psi_i|\sum_{i=1}^2 B_{i,\lambda}|\psi_i\rangle - \langle\varphi_i|\sum_{i=1}^2 B_{i,\lambda}|\varphi_i\rangle)}. \quad (4.32)$$

The full protocol on $\mathcal{H}_{\text{Baths}} \otimes \mathcal{H}_C \otimes \mathcal{H}_W$ is $U_{\text{opt,nc}}^{(\lambda)}(\mathbf{Q}_\lambda) \otimes I_C$. As with the commutative case, the cyclicity and no-cheating condition hold. Further, the average conservation B1* is satisfied, though the strict conservation is not necessarily. Especially, the final state $\rho_{\text{opt,nc}}^{(\lambda)} = \text{tr}_{\mathcal{H}_W} U_{\text{opt,nc}}^{(\lambda)}(\mathbf{Q}_\lambda)(\tau_{\theta_0}^{(\lambda)} \otimes \rho_W)U_{\text{opt,nc}}^{(\lambda)}(\mathbf{Q}_\lambda)^\dagger$ does not depend on the state of the battery.

As the achievement of FGCB in this case, we show the following non-commutative version of Theorem 4.1:

Theorem 4.2. *Let $A_{i,\lambda}$ and $B_{i,\lambda}$ be not necessarily commutative. Let Assumption 4.1 be satisfied. For any $\mathbf{Q}_\lambda = (\Delta Q_{A,2,\lambda}, \Delta Q_{B,1,\lambda}, \Delta Q_{B,2,\lambda})$, there exists a generalized heat engine implementing $U_{\text{opt,nc}}^{(\lambda)}(\mathbf{Q}_\lambda) \otimes I_C$ in the sense of the semi-explicit battery formulation B1*, B2-B4. Especially, the final state $\rho_{\text{opt,nc}}^{(\lambda)} = \text{tr}_{\mathcal{H}_W} U_{\text{opt,nc}}^{(\lambda)}(\mathbf{Q}_\lambda)(\tau_{\theta_0}^{(\lambda)} \otimes \rho_W)U_{\text{opt,nc}}^{(\lambda)}(\mathbf{Q}_\lambda)^\dagger$ of the baths is independent of the initial state of the battery ρ_W . If \mathbf{Q}_λ satisfies (4.16), then the final state $\rho_{\text{opt,nc}}^{(\lambda)}$ of the baths satisfies*

$$\text{tr} A_{i,\lambda} \rho_{\text{opt,nc}}^{(\lambda)} = \text{tr} A_{i,\lambda} \tau_{\theta_\lambda}^{(\lambda)} + o\left(\frac{\|\mathbf{Q}_\lambda\|^2}{\lambda}\right) \quad (4.33)$$

$$\text{tr} B_{i,\lambda} \rho_{\text{opt,nc}}^{(\lambda)} = \text{tr} B_{i,\lambda} \tau_{\theta_\lambda}^{(\lambda)} + o\left(\frac{\|\mathbf{Q}_\lambda\|^2}{\lambda}\right) \quad (i = 1, 2). \quad (4.34)$$

Hence, FGCB is asymptotically achieved up to $o\left(\frac{\|\mathbf{Q}_\lambda\|^2}{\lambda}\right)$ by this engine.

The statement is the same as Theorem 4.1 except the construction of the protocol $U_{\text{opt,nc}}^{(\lambda)}(\mathbf{Q}_\lambda)$ and its final state $\rho_{\text{opt,nc}}^{(\lambda)}$, and the average conservation law B1*. We prove Theorem 4.2 in a similar way to Theorem 4.1 by taking care of non-commutativity. Proof is also done in Sec. 8.

As with the commutative case, achievability of FGCB immediately follows from Theorem 4.2 as follows:

Corollary 4.2. *Under Assumption 4.1 and (4.16), the generalized heat of the heat engine implementing the operation $U_{\text{opt,nc}}^{(\lambda)}(\mathbf{Q}_\lambda) \otimes I_C$ coincides with \mathbf{Q}_λ up to $o\left(\frac{\|\mathbf{Q}_\lambda\|^2}{\lambda}\right)$ as follows:*

$$\text{tr} A_{2,\lambda}(\tau_{\theta_0}^{(\lambda)} - \rho_{\text{opt,nc}}^{(\lambda)}) = \Delta Q_{A,2,\lambda} + o\left(\frac{\|\mathbf{Q}_\lambda\|^2}{\lambda}\right) \quad (4.35)$$

$$\text{tr} B_{i,\lambda}(\tau_{\theta_0}^{(\lambda)} - \rho_{\text{opt,nc}}^{(\lambda)}) = \Delta Q_{B,i,\lambda} + o\left(\frac{\|\mathbf{Q}_\lambda\|^2}{\lambda}\right) \quad (i = 1, 2). \quad (4.36)$$

Up to $o\left(\frac{\|\mathbf{Q}_\lambda\|^2}{\lambda}\right)$, the work output of Quantity A of this engine equals to the maximum work with the generalized heat \mathbf{Q}_λ as follows:

$$\Delta W_A = \text{tr}(A_{1,\lambda} + A_{2,\lambda})(\tau_{\theta_0}^{(\lambda)} - \rho_{\text{opt,nc}}^{(\lambda)}) = \Delta W_{A,\lambda}^{\text{opt}}(\mathbf{Q}_\lambda) + o\left(\frac{\|\mathbf{Q}_\lambda\|^2}{\lambda}\right). \quad (4.37)$$

Hence, FGCB is asymptotically achieved up to $o\left(\frac{\|\mathbf{Q}_\lambda\|^2}{\lambda}\right)$ by this engine.

5 A generalization of the central limit theorem

In this section, we show the following generalization of the central limit theorem to apply it to the thermal state satisfying Assumption 2.1. This is needed to verify the strong large deviation theorem (Lemma 6.1) in the next section.

Let $(X_\lambda)_{\lambda \in \Lambda}$ be a family of random variables with each finite sample space Ω_λ , where Λ is the set of all positive real numbers or all positive integers. Let $M_\lambda(t) := \mathbb{E}[e^{tX_\lambda}]$ be the moment generating function, and $\psi_\lambda(t) := \log \mathbb{E}[e^{tX_\lambda}]$ be the cumulant generating function (cgf) of X_λ , where \mathbb{E} denotes the expectation value. We denote the cumulative distribution function (cdf) of $(X_\lambda - \mathbb{E}[X_\lambda])/\sigma_\lambda$ by $F_\lambda(x) := \mathbb{P}\left(\frac{X_\lambda - \mathbb{E}[X_\lambda]}{\sigma_\lambda} \leq x\right)$, where σ_λ is the standard deviation of X_λ . We use the following lemma [40, Lemma 2, pp. 538]:

Lemma 5.1 (Feller [40]). *Let F be a probability distribution whose expectation value is 0. Let φ be the characteristic function*

$$\varphi(\zeta) := \int_{-\infty}^{\infty} e^{i\zeta x} F(dx) \quad (5.1)$$

of F . Let \mathcal{N} be the cumulative distribution function of the standard Gaussian distribution. Then,

$$|F(x) - \mathcal{N}(x)| \leq \int_{-T}^T \left| \frac{\varphi(\zeta) - e^{-\frac{1}{2}\zeta^2}}{\zeta} \right| d\zeta + \frac{24m}{T} \quad (5.2)$$

holds for any $x \in \mathbb{R}$, $T > 0$ and $m \geq 1/\sqrt{2\pi}$.

Then, we give the following generalization of the central limit theorem.

Theorem 5.1. *If the cgf asymptotically satisfies*

$$\psi_\lambda(t) = \lambda\psi(t) + o(\lambda) \quad (5.3)$$

pointwise with a function $\psi(t)$ on some interval $I := [a_1, a_2] \ni 0$, the following asymptotic expansion uniformly holds for large enough λ :

$$F_\lambda(x) = \mathcal{N}(x) + \mathcal{O}\left(\lambda^{-\frac{1}{2}}\right). \quad (5.4)$$

Proof. Step1: In this step, applying the method by Curtiss [41], we prove that the cgf ψ_λ is extended to a holomorphic function on a small region around the real axis independently of λ . In addition, we show that this holomorphic function satisfies (5.3) uniformly on this region.

We set $\mathbb{E}[X_\lambda] = 0$ without loss of generality. Then, since M_λ is convex, it takes the maximum on I at a_1 or a_2 . By (5.3), because $M_\lambda(t_0)^{\lambda^{-1}}$ converges to $e^{\psi(t_0)}$ for fixed $t_0 = a_1$ or a_2 , $M_\lambda(t)^{\lambda^{-1}}$ is uniformly bounded on $t \in I$. Because of

$$|M_\lambda(t + i\zeta)| := |\mathbb{E}[e^{(t+i\zeta)X_\lambda}]| \leq \mathbb{E}[|e^{(t+i\zeta)X_\lambda}|] = \mathbb{E}[e^{tX_\lambda}] = M_\lambda(t) \quad (\forall \zeta \in \mathbb{R}), \quad (5.5)$$

$M_\lambda(z)^{\lambda^{-1}}$ is uniformly bounded on the strip $\mathcal{S} := \{z \in \mathbb{C} | \operatorname{Re} z \in I\}$. Thus, by Vitali's theorem, there exists a holomorphic function $m(z)$ such that $\lim_{\lambda \rightarrow \infty} M_\lambda(z)^{\lambda^{-1}} = m(z)$ uniformly in any bounded closed subregion of \mathcal{S} . Since $m(t) = e^{\psi(t)} > 0$ ($t \in I$), $\operatorname{Re} m(z) > 0$ ($z \in B_{\tilde{\delta}} := \{z \in \mathbb{C} | |z| \leq \tilde{\delta}\}$) holds for

sufficiently small $\tilde{\delta} > 0$. Thus, $\psi(z) := \log m(z)$ is well defined as a holomorphic function on $B_{\tilde{\delta}}$. Because $M_\lambda(z)^{\lambda^{-1}}$ converges uniformly to $m(z)$ on $B_{\tilde{\delta}}$, the relation $\operatorname{Re} M_\lambda(z)^{\lambda^{-1}} > 0$ ($z \in B_{\tilde{\delta}}$) holds for sufficiently large λ , hence the relation $\operatorname{Re} M_\lambda(z) > 0$ does. Hence, $\psi_\lambda(z) := \log M_\lambda(z)$ is similarly well defined as a holomorphic function on $B_{\tilde{\delta}}$. Hence, $\psi_\lambda^{(n)}(z) = \lambda\psi^{(n)}(z) + o(\lambda)$ holds for any n , where $f^{(n)}$ denotes the n -th derivative of f . Especially, we have

$$\sigma_\lambda^2 = \psi_\lambda''(0) = \lambda\psi''(0) + o(\lambda) = \mathcal{O}(\lambda). \quad (5.6)$$

Step 2: In this step, combining the estimations in [40] and the asymptotic behavior of the cgf, we establish the desired estimation (5.4).

The quantity $|\psi^{(3)}(z)|$ has the maximum value on $B_{\tilde{\delta}}$ since $\psi^{(3)}(z)$ is holomorphic. Thus, because of $|\psi_\lambda^{(3)}(z)| = |\lambda\psi^{(3)}(z) + o(\lambda)| \leq \lambda(|\psi^{(3)}(z)| + o(1))$, there exists $C_0 > 0$ such that

$$|\psi_\lambda^{(3)}(z)| \leq 6C_0\lambda \quad (z \in B_{\tilde{\delta}}) \quad (5.7)$$

holds for large enough λ . Then, we take a $\delta > 0$ as

$$\delta < \min \left\{ \tilde{\delta}, \frac{\psi''(0)}{8C_0} \right\} < \frac{\psi_\lambda''(0)}{4C_0\lambda} = \frac{\sigma_\lambda^2}{4C_0\lambda}, \quad (5.8)$$

where the last inequality holds for sufficiently large λ . Since F_λ is the distribution function of X_λ/σ_λ , the characteristic function $\varphi_\lambda(\zeta)$ of F_λ is equal to $M_\lambda(i\zeta/\sigma_\lambda)$ since M_λ is analytically continued on \mathcal{S} . In addition, because $\psi_\lambda = \log M_\lambda$ is analytically continued on $B_{\tilde{\delta}}$, we have $\varphi_\lambda(\zeta) = e^{\psi_\lambda(i\zeta/\sigma_\lambda)}$ for any ζ such that $|\zeta|/\sigma_\lambda \leq \delta < \tilde{\delta}$. Applying Lemma 5.1 with $T = \delta\sigma_\lambda$ and $m = 1$, we have

$$|F_\lambda(x) - \mathcal{N}(x)| \leq \int_{-\delta\sigma_\lambda}^{\delta\sigma_\lambda} \left| \frac{e^{\psi_\lambda\left(\frac{i\zeta}{\sigma_\lambda}\right)} - e^{-\frac{1}{2}\zeta^2}}{\zeta} \right| d\zeta + \frac{C}{\sigma_\lambda} \quad (5.9)$$

with a constant $C := 24/\delta$. The second term is $\mathcal{O}\left(\lambda^{-\frac{1}{2}}\right)$ from (5.6). Then, we apply a similar method to [40, pp. 534]. Observing that $|e^\alpha - 1| \leq |\alpha|e^\gamma$ for any $\gamma \geq |\alpha|$, we have

$$\left| e^{\psi_\lambda\left(\frac{i\zeta}{\sigma_\lambda}\right) + \frac{1}{2}\zeta^2} - 1 \right| \leq \left| \psi_\lambda\left(\frac{i\zeta}{\sigma_\lambda}\right) + \frac{1}{2}\zeta^2 \right| e^\gamma \quad (5.10)$$

for any $\gamma \geq \left| \psi_\lambda\left(\frac{i\zeta}{\sigma_\lambda}\right) + \frac{1}{2}\zeta^2 \right|$. By the Taylor expansion of ψ_λ around 0 for $i\zeta/\sigma_\lambda$ where $|\zeta| \leq \delta\sigma_\lambda$, there exists $\theta_\lambda \in B_{|\zeta|/\sigma_\lambda} \subset B_\delta \subset B_{\tilde{\delta}}$ such that

$$\left| \psi_\lambda\left(\frac{i\zeta}{\sigma_\lambda}\right) + \frac{1}{2}\zeta^2 \right| = \frac{1}{6} \left| \psi_\lambda^{(3)}(\theta_\lambda) \right| \frac{|\zeta|^3}{\sigma_\lambda^3}. \quad (5.11)$$

Since we focus on the domain $|\zeta| \leq \delta\sigma_\lambda$ of the integral in (5.9), we have

$$\frac{1}{6} \left| \psi_\lambda^{(3)}(\theta_\lambda) \right| \frac{|\zeta|^3}{\sigma_\lambda^3} \stackrel{(a)}{\leq} \lambda C_0 \frac{|\zeta|^3}{\sigma_\lambda^3} \leq \lambda C_0 \delta \frac{|\zeta|^2}{\sigma_\lambda^2} \stackrel{(b)}{\leq} \frac{1}{4} |\zeta|^2 \quad (5.12)$$

for large enough λ , where (a) and (b) follow from (5.7) and (5.8) respectively. Thus, we can take $\gamma = \frac{1}{4}|\zeta|^2$ in (5.10). Applying the first inequality in (5.12) combined with (5.10), we have the following estimation of the integral in (5.9) as

$$\int_{-\delta\sigma_\lambda}^{\delta\sigma_\lambda} \left| \frac{e^{\psi_\lambda\left(\frac{i\zeta}{\sigma_\lambda}\right)} - e^{-\frac{1}{2}\zeta^2}}{\zeta} \right| d\zeta \leq \lambda C_0 \sigma_\lambda^{-3} \int_{-\delta\sigma_\lambda}^{\delta\sigma_\lambda} \zeta^2 e^{-\frac{1}{2}\zeta^2} d\zeta \leq \lambda C_0 \sigma_\lambda^{-3} \int_{-\infty}^{\infty} \zeta^2 e^{-\frac{1}{2}\zeta^2} d\zeta = \mathcal{O}\left(\lambda^{-\frac{1}{2}}\right) \quad (5.13)$$

since (5.6) holds, and the Gaussian integral is finite. Thus, $|F_\lambda(x) - \mathcal{N}(x)| = \mathcal{O}\left(\lambda^{-\frac{1}{2}}\right)$ is proved. \square

6 Strong large deviation for the number of states

In this section, we prepare a key lemma (Lemma 6.1) to deal with the estimation of the relative entropy for the proof of Theorems 4.1 and 4.2. Here, as in Sec. 4, we assume Assumption 4.1, i.e. the asymptotic extensivity of the free entropy ϕ_λ of the thermal states $\tau_\theta^{(\lambda)}$ (Definition 2.1) and its derivatives. Let ν be the asymptotic density $\nu := -(\sum_{i=1}^4 \eta_i(\theta_0)\theta_0^i + \phi(\theta_0))$ of the negative entropy of the initial thermal state $\tau_{\theta_0}^{(\lambda)}$. Recall that the probability distributions $p_{\theta_0}^{(\lambda)}$ and $p_{\theta_\lambda}^{(\lambda)}$ are defined in (4.4) (commutative case), (4.30) and (4.31) (non-commutative case) as the eigenvalues of the density matrices of the thermal states, where θ_λ is defined by (3.23)-(3.26) with a vector $\mathbf{Q}_\lambda = (\Delta Q_{A,2,\lambda}, \Delta Q_{B,1,\lambda}, \Delta Q_{B,2,\lambda})$ in the main text. We assume $\lambda^{-\frac{5}{8}} \ll \|\mathbf{Q}_\lambda\| \ll \lambda$ as in Theorems 4.1 and 4.2. For our purpose, we need a detailed estimation of the number of states $N_l^{(\lambda)}(a)$ ($l = 0, 1$) ($a \in \mathbb{R}$) defined as

$$N_l^{(\lambda)}(a) := \begin{cases} \# \left\{ j \mid \frac{1}{\lambda} \log p_{\theta_0}^{(\lambda)}(j) \geq \nu + \lambda^{-\frac{1}{2}} a \right\} & (l = 0) \\ \# \left\{ j \mid \frac{1}{\lambda} \log p_{\theta_\lambda}^{(\lambda)}(j) \geq \nu + \lambda^{-\frac{1}{2}} a \right\} & (l = 1). \end{cases} \quad (6.1)$$

We carry out the estimation of $N_l^{(\lambda)}(a)$ by slightly modifying the strong large deviation theorem by Joutard [42].

We firstly prepare some notations and results needed for the estimation along the line of [42]. We regard $\lambda^{-1} \log p_{\theta_0}^{(\lambda)}$ and $\lambda^{-1} \log p_{\theta_\lambda}^{(\lambda)}$ as the random variables $Z_{0,\lambda}(j) := \lambda^{-1} \log p_{\theta_0}^{(\lambda)}(j)$ and $Z_{1,\lambda}(j) := \lambda^{-1} \log p_{\theta_\lambda}^{(\lambda)}(j)$ ($j \in \mathbb{N}_{d_\lambda}$) which are uniformly distributed on \mathbb{N}_{d_λ} . We denote the distribution function of $\lambda Z_{l,\lambda}$ by $K_{l,\lambda}$. Let $\varphi_{l,\lambda}$ ($l = 0, 1$) be the normalized cgf of $\lambda Z_{l,\lambda}$,

$$\varphi_{l,\lambda}(t) := \lambda^{-1} \log \mathbb{E}[e^{t\lambda Z_{l,\lambda}}] = \lambda^{-1} \log \sum_{j \in \mathbb{N}_{d_\lambda}} \frac{1}{d_\lambda} e^{t\lambda Z_{l,\lambda}(j)}. \quad (6.2)$$

They have other expressions

$$\varphi_{0,\lambda}(t) = \lambda^{-1} (\phi_\lambda(t\theta_0) - t\phi_\lambda(\theta_0)) - \lambda^{-1} \log d_\lambda \quad (6.3)$$

$$\varphi_{1,\lambda}(t) = \lambda^{-1} (\phi_\lambda(t\theta_\lambda) - t\phi_\lambda(\theta_\lambda)) - \lambda^{-1} \log d_\lambda. \quad (6.4)$$

Then, by Assumption 4.1, there exists an interval I_1 including 1 such that both of $\varphi_{l,\lambda}(t) + \lambda^{-1} \log d_\lambda$ ($l = 0, 1$) converge to $\varphi(t) := \phi(t\theta_0) - t\phi(\theta_0)$ uniformly with respect to t on I_1 . Then, we define $\Lambda_\lambda(t) := \lambda^{-1} \sum_{i,j} t[\eta_i(t\theta_0) - \eta_i(\theta_0)]g^{ij}(\theta_0)y_{\lambda,j}$, $(y_{\lambda,1}, y_{\lambda,2}, y_{\lambda,3}, y_{\lambda,4}) := \boldsymbol{\eta}_\lambda(\theta_\lambda) - \boldsymbol{\eta}_\lambda(\theta_0)$, where $\boldsymbol{\eta}_\lambda$ is defined in (2.3). Since φ is strictly convex, $f(x) := (\varphi')^{-1}(x)$ is well defined.

The first and second derivatives of $\varphi_{1,\lambda}$ are related with those of $\varphi_{0,\lambda}$ by using the Taylor expansion and the expressions (6.3) and (6.4) as

$$\varphi'_{1,\lambda}(t) = \varphi'_{0,\lambda}(t) + \Lambda'_\lambda(t) + \mathcal{O}\left(\lambda^{-\frac{1}{2}}\right) + \mathcal{O}\left(\frac{\|\mathbf{Q}_\lambda\|^2}{\lambda^2}\right) \quad (6.5)$$

$$\varphi'_{1,\lambda}(1) = \lambda^{-1}\left[-\sum_i \eta_{\lambda,i}(\boldsymbol{\theta}_\lambda)\theta_\lambda^i - \phi_\lambda(\boldsymbol{\theta}_\lambda)\right] = -S(\tau_{\boldsymbol{\theta}_\lambda}^{(\lambda)}) = -S(\tau_{\boldsymbol{\theta}_0}^{(\lambda)}) = \varphi'_{0,\lambda}(1) \quad (6.6)$$

$$\varphi''_{1,\lambda}(t) = \varphi''_{0,\lambda}(t) + \Lambda''_\lambda(t) + \mathcal{O}\left(\lambda^{-\frac{1}{2}}\right) + \mathcal{O}\left(\frac{\|\mathbf{Q}_\lambda\|^2}{\lambda^2}\right). \quad (6.7)$$

Now, we give an asymptotic expansion of $N_l^{(\lambda)}(a)$ through a strong large deviation estimation of the upper tail probability $\mathbb{P}(Z_{l,\lambda} \geq \nu + \lambda^{-\frac{1}{2}}a) = d_\lambda^{-1}N_l^{(\lambda)}(a)$ in the same way as [42].

Lemma 6.1. *Let $\lambda^{-\frac{5}{8}} \ll \|\mathbf{Q}_\lambda\| \ll \lambda$ and Assumption 4.1 be satisfied. Then, for any $a \in \mathbb{R}$ and sufficiently large λ , defining $r_{k,\lambda}^l$ ($l = 0, 1$), ($k = 0, 1, 2$) by*

$$r_{2,\lambda}^1 := \frac{1}{2}\varphi'_{0,\lambda}(1)f''(\nu) + \frac{1}{2}\varphi''_{0,\lambda}(1)f'(\nu)^2 - f'(\nu) - \frac{1}{2}\nu f''(\nu) + \frac{1}{2}\Lambda''_\lambda(1)f'(\nu)^2 \quad (6.8)$$

$$r_{1,\lambda}^1 := [\varphi'_{0,\lambda}(1)f'(\nu) - \nu f'(\nu) - 1 + \varphi''(1)^{-1}(\nu - \varphi'_{0,\lambda}(1))\Lambda''_\lambda(1)f'(\nu)]\lambda^{\frac{1}{2}} \quad (6.9)$$

$$\begin{aligned} r_{0,\lambda}^1 := & -\lambda\nu - \frac{1}{2}\varphi''(1)^{-1}(\nu - \varphi'_{0,\lambda}(1))^2\lambda - \log\sqrt{2\pi} - \frac{1}{2}\log\varphi''(1) - \frac{1}{2}\log\lambda \\ & + \frac{1}{2}\varphi''(1)^{-2}\Lambda''_\lambda(1)(\nu - \varphi'_{0,\lambda}(1))^2\lambda - \frac{1}{2\varphi''(1)}\Lambda''_\lambda(1) \end{aligned} \quad (6.10)$$

$$r_{2,\lambda}^0 := \frac{1}{2}\varphi'_{0,\lambda}(1)f''(\nu) + \frac{1}{2}\varphi''_{0,\lambda}(1)f'(\nu)^2 - f'(\nu) - \frac{1}{2}\nu f''(\nu) \quad (6.11)$$

$$r_{1,\lambda}^0 := [\varphi'_{0,\lambda}(1)f'(\nu) - \nu f'(\nu) - 1]\lambda^{\frac{1}{2}} \quad (6.12)$$

$$r_{0,\lambda}^0 := -\lambda\nu - \frac{1}{2}\varphi''(1)^{-1}(\nu - \varphi'_{0,\lambda}(1))^2\lambda - \log\sqrt{2\pi} - \frac{1}{2}\log\varphi''(1) - \frac{1}{2}\log\lambda, \quad (6.13)$$

we have

$$N_1^{(\lambda)}(a) = \exp\left[r_{2,\lambda}^1 a^2 + r_{1,\lambda}^1 a + r_{0,\lambda}^1 + \mathcal{O}\left(\lambda^{-\frac{1}{2}}\right) + \mathcal{O}\left(\lambda^{-2}\|\mathbf{Q}_\lambda\|^2\right)\right]. \quad (6.14)$$

$$N_0^{(\lambda)}(a) = \exp\left[r_{2,\lambda}^0 a^2 + r_{1,\lambda}^0 a + r_{0,\lambda}^0 + \mathcal{O}\left(\lambda^{-\frac{1}{2}}\right)\right]. \quad (6.15)$$

Remark 6.1. *Joutard gave the strong large deviation theorem (Theorem 1 of [42]) under his assumptions (A.1) and (A.2) in [42]. The latter (A.2) is the Edgeworth expansion, which is also satisfied in our case up to the first order. However, the former (A.1) requires that there exist functions φ_l , J_l independently of λ such that*

$$\varphi'_{l,\lambda}(t) = \varphi'_l(t) + \lambda^{-1}J_l(t) + o(\lambda^{-1}). \quad (6.16)$$

Because of $\Lambda'_\lambda(t) = \mathcal{O}(\lambda^{-1}\|\mathbf{Q}_\lambda\|)$ and $\lambda^{\frac{5}{8}} \ll \|\mathbf{Q}_\lambda\|$, $\Lambda'_\lambda(t)$ has strictly larger order than λ^{-1} . Hence, (6.5) contradicts (6.16). As for $\varphi'_{0,\lambda}$, because just

$$\varphi'_{0,\lambda}(t) = \varphi'(t) + \mathcal{O}(\lambda^{\alpha-1}) \quad (6.17)$$

is guaranteed, (6.16) is not necessarily satisfied. In addition, he only treated the tail probability of the form $\mathbb{P}(Z_\lambda \geq a)$, where a does not depend on the scale λ . In our case, a is replaced by $\nu + \lambda^{-\frac{1}{2}}a$. Hence, we cannot directly apply Theorem 1 of [42] for our situation. We will slightly modify his proof to obtain Lemma 6.1.

For the proof of Lemma 6.1, we prepare several lemmas.

Lemma 6.2.

$$\nu - \varphi'_{0,\lambda}(1) = \mathcal{O}(\lambda^{\alpha-1}) = o(\lambda^{-\frac{1}{2}}) \quad (6.18)$$

$$1 - \varphi''_{0,\lambda}(1)f'(\nu) = \mathcal{O}(\lambda^{\alpha-1}) = o(\lambda^{-\frac{1}{2}}) \quad (6.19)$$

$$\Lambda''_\lambda(1) = \mathcal{O}(\lambda^{-1}\|\mathbf{Q}_\lambda\|) = o(1). \quad (6.20)$$

Proof. These relations follow from Assumption 4.1 and $\|\mathbf{Q}_\lambda\| = o(\lambda)$, \square

We focus on $t_{\lambda,a} := f(\nu + \lambda^{-\frac{1}{2}}a)$ as the variable t . Using the exponential tilting of the measure, we define the random variable $\lambda Z_{l,\lambda}^*$ whose distribution function is $K_{l,\lambda}^*$ ($l = 0, 1$) which is defined as

$$K_{l,\lambda}^*(u) := \int_{-\infty < x \leq u} \exp[xt_{\lambda,a} - \lambda\varphi_{l,\lambda}(t_{\lambda,a})] dK_{l,\lambda}(x). \quad (6.21)$$

In fact, it is a distribution function since

$$\lim_{u \rightarrow \infty} K_{l,\lambda}^*(u) = \int_{-\infty < x < \infty} \exp[xt_{\lambda,a} - \lambda\varphi_{l,\lambda}(t_{\lambda,a})] dK_{l,\lambda}(x) = \frac{\mathbb{E}[e^{t\lambda Z_{l,\lambda}}]}{\mathbb{E}[e^{t\lambda Z_{l,\lambda}}]} = 1 \quad (6.22)$$

and the other conditions are trivially satisfied. Since the mean and the variance of $\lambda Z_{l,\lambda}^*$ are respectively equal to $\lambda\varphi'_{l,\lambda}(t_{\lambda,a})$ and $\varphi''_{l,\lambda}(t_{\lambda,a})$, we define the standardized random variable $V_{l,\lambda}$ as

$$V_{l,\lambda} := \frac{\lambda Z_{l,\lambda}^* - \lambda\varphi'_{l,\lambda}(t_{\lambda,a})}{\sqrt{\lambda\varphi''_{l,\lambda}(t_{\lambda,a})}}. \quad (6.23)$$

Then, we have the following lemma.

Lemma 6.3. *The distribution function $F_{l,\lambda}$ of the random variable $V_{l,\lambda}$ ($l = 0, 1$) satisfies the central limit theorem as*

$$\sup_{y \in \mathbb{R}} |F_{l,\lambda}(y) - \mathcal{N}(y)| = \mathcal{O}\left(\lambda^{-\frac{1}{2}}\right). \quad (6.24)$$

Proof. The cgf $\psi_{l,\lambda}(s)$ of $\lambda Z_{l,\lambda}^*$ is calculated as

$$\psi_{l,\lambda}(s) = \log \int_{-\infty < u < \infty} e^{su} dK_{l,\lambda}^*(u) = \log \int_{-\infty < u < \infty} e^{(s+t_{\lambda,a})u - \lambda\varphi_{l,\lambda}(t_{\lambda,a})} dK_{l,\lambda}(u) = \lambda\varphi_{l,\lambda}(s + t_{\lambda,a}) - \lambda\varphi_{l,\lambda}(t_{\lambda,a}). \quad (6.25)$$

As for $l = 1$, (6.4) and (6.25) yield

$$\psi_{1,\lambda}(s) = \phi_\lambda((s + t_{\lambda,a})\boldsymbol{\theta}_\lambda) - (s + t_{\lambda,a})\phi_\lambda(\boldsymbol{\theta}_\lambda) - (\phi_\lambda(t_{\lambda,a}\boldsymbol{\theta}_\lambda) - t_{\lambda,a}\phi_\lambda(\boldsymbol{\theta}_\lambda)) = \phi_\lambda((s + t_{\lambda,a})\boldsymbol{\theta}_\lambda) - (s + t_{\lambda,a})\phi_\lambda(\boldsymbol{\theta}_\lambda). \quad (6.26)$$

Thus, because of Assumption 4.1, (6.29) and the definition of $\boldsymbol{\theta}_\lambda$, there exists a small interval $I_0 \ni 0$ such that

$$\psi_{1,\lambda}(s) = \lambda[\phi((s+1)\boldsymbol{\theta}_0) - (s+1)\phi(\boldsymbol{\theta}_0)] + o(\lambda) \quad (6.27)$$

holds for any $s \in I_0$. In the same way, we also have

$$\psi_{0,\lambda}(s) = \lambda[\phi((s+1)\boldsymbol{\theta}_0) - (s+1)\phi(\boldsymbol{\theta}_0)] + o(\lambda). \quad (6.28)$$

Therefore, both $\lambda Z_{l,\lambda}$ ($l = 0, 1$) satisfy the condition of Theorem 5.1. Hence the distribution functions $F_{l,\lambda}$ of their standardized random variable $V_{l,\lambda}$ satisfy the central limit theorem (6.24) by Theorem 5.1. \square

Proof of Lemma 6.1. Step 1: First, we prepare several formulas for $t_{\lambda,a}$ and $\varphi_{l,\lambda}$ together with its derivatives. The Taylor expansion with (6.3), (6.4) yields

$$t_{\lambda,a} = 1 + f'(\nu)a\lambda^{-\frac{1}{2}} + \frac{1}{2}f''(\nu)a^2\lambda^{-1} + \mathcal{O}(\lambda^{-\frac{3}{2}}), \quad (6.29)$$

$$\begin{aligned} \varphi_{l,\lambda}(t_{\lambda,a}) &= \varphi_{l,\lambda}(1) + \varphi'_{l,\lambda}(1)[\lambda^{-\frac{1}{2}}f'(\nu)a + \frac{1}{2}\lambda^{-1}f''(\nu)a^2] + \frac{1}{2}\varphi''_{l,\lambda}(1)\lambda^{-1}f'(\nu)^2a^2 + \mathcal{O}(\lambda^{-\frac{3}{2}}) \\ &= -\lambda^{-1}\log d_\lambda + \lambda^{-\frac{1}{2}}\varphi'_{l,\lambda}(1)f'(\nu)a + \frac{1}{2}\lambda^{-1}[\varphi'_{l,\lambda}(1)f''(\nu)a^2 + \varphi''_{l,\lambda}(1)f'(\nu)^2a^2] + \mathcal{O}(\lambda^{-\frac{3}{2}}). \end{aligned} \quad (6.30)$$

Furthermore, the Taylor expansion gives

$$\begin{aligned} \varphi'_{1,\lambda}(t_{\lambda,a}) &= \varphi'_{1,\lambda}(1) + \lambda^{-\frac{1}{2}}\varphi''_{1,\lambda}(1)f'(\nu)a + \mathcal{O}(\lambda^{-1}) \\ &\stackrel{(a)}{=} \varphi'_{0,\lambda}(1) + \lambda^{-\frac{1}{2}}[\varphi''_{0,\lambda}(1) + \Lambda''_\lambda(1)]f'(\nu)a + \mathcal{O}(\lambda^{-1}) \end{aligned} \quad (6.31)$$

$$\begin{aligned} \varphi''_{1,\lambda}(t_{\lambda,a}) &= \varphi''_{1,\lambda}(1) + \mathcal{O}(\lambda^{-\frac{1}{2}}) \\ &\stackrel{(b)}{=} \varphi''_{0,\lambda}(1) + \Lambda''_\lambda(1) + \mathcal{O}(\lambda^{-\frac{1}{2}}), \end{aligned} \quad (6.32)$$

where (a) follows from (6.5) and (6.6), and (b) follows from (6.7). Here, we calculated (6.30), (6.31), and (6.32) up to the necessary orders for the later analysis. In the same way, we have

$$\varphi'_{0,\lambda}(t_{\lambda,a}) = \varphi'_{0,\lambda}(1) + \lambda^{-\frac{1}{2}}\varphi''_{0,\lambda}(1)f'(\nu)a + \mathcal{O}(\lambda^{-1}) \quad (6.33)$$

$$\varphi''_{0,\lambda}(t_{\lambda,a}) = \varphi''_{0,\lambda}(1) + \mathcal{O}(\lambda^{-\frac{1}{2}}). \quad (6.34)$$

Also, applying (6.29), (6.32) and (6.34), we have the asymptotic expansions for $u_{l,\lambda} := t_{\lambda,a}\sqrt{\lambda\varphi''_{l,\lambda}(t_{\lambda,a})}$ as

$$\log u_{1,\lambda} = \frac{1}{2}\log \varphi''(1) + \frac{1}{2\varphi''(1)}\Lambda''_\lambda(1) + \frac{1}{2}\log \lambda + \mathcal{O}(\lambda^{-\frac{1}{2}}) + \mathcal{O}(\lambda^{-2}\|\mathbf{Q}_\lambda\|^2), \quad (6.35)$$

$$\log u_{0,\lambda} = \frac{1}{2}\log \varphi''(1) + \frac{1}{2}\log \lambda + \mathcal{O}(\lambda^{-\frac{1}{2}}) + \mathcal{O}(\lambda^{-2}\|\mathbf{Q}_\lambda\|^2). \quad (6.36)$$

Step 2: In this step, we divide the probability $\mathbb{P}(Z_{l,\lambda} \geq \nu + \lambda^{-\frac{1}{2}}a)$ into two parts to estimate it. Defining

$$b_{l,\lambda} := \lambda t_{\lambda,a} (\varphi'_{l,\lambda}(t_{\lambda,a}) - (\nu + \lambda^{-\frac{1}{2}}a)) \quad (6.37)$$

$$c_{l,\lambda} := \frac{\sqrt{\lambda}(\nu + \lambda^{-\frac{1}{2}}a - \varphi'_{l,\lambda}(t_{\lambda,a}))}{\sqrt{\varphi''_{l,\lambda}(t_{\lambda,a})}} \quad (6.38)$$

we calculate the probability $\mathbb{P}(Z_{l,\lambda} \geq \nu + \lambda^{-\frac{1}{2}}a)$ as

$$\begin{aligned} & \mathbb{P}(Z_{l,\lambda} \geq \nu + \lambda^{-\frac{1}{2}}a) \\ &= \int_{u \geq \lambda(\nu + \lambda^{-\frac{1}{2}}a)} dK_{l,\lambda}(u) \\ &= \int_{u \geq \lambda(\nu + \lambda^{-\frac{1}{2}}a)} e^{-ut_{\lambda,a} + \lambda\varphi_{l,\lambda}(t_{\lambda,a})} e^{ut_{\lambda,a} - \lambda\varphi_{l,\lambda}(t_{\lambda,a})} dK_{l,\lambda}(u) \\ &= \int_{u \geq \lambda(\nu + \lambda^{-\frac{1}{2}}a)} e^{-ut_{\lambda,a} + \lambda\varphi_{l,\lambda}(t_{\lambda,a})} dK_{l,\lambda}^*(u) \\ &= e^{\lambda[\varphi_{l,\lambda}(t_{\lambda,a}) - t_{\lambda,a}\varphi'_{l,\lambda}(t_{\lambda,a})]} \int_{u \geq \lambda(\nu + \lambda^{-\frac{1}{2}}a)} e^{-ut_{\lambda,a} + \lambda\varphi_{l,\lambda}(t_{\lambda,a})} dK_{l,\lambda}^*(u) \\ &\stackrel{(a)}{=} e^{\lambda[\varphi_{l,\lambda}(t_{\lambda,a}) - t_{\lambda,a}(\nu + \lambda^{-\frac{1}{2}}a)]} e^{-\lambda t_{\lambda,a}(\varphi'_{l,\lambda}(t_{\lambda,a}) - (\nu + \lambda^{-\frac{1}{2}}a))} \int_{y \geq c_{l,\lambda}} e^{-u_{l,\lambda}y} dF_{l,\lambda}(y) \\ &= e^{\lambda[\varphi_{l,\lambda}(t_{\lambda,a}) - t_{\lambda,a}(\nu + \lambda^{-\frac{1}{2}}a)]} e^{-b_{l,\lambda}} \int_{y \geq c_{l,\lambda}} e^{-u_{l,\lambda}y} dF_{l,\lambda}(y), \end{aligned} \quad (6.39)$$

where the equality (a) follows from integration by substitution with $y = (u - \lambda\varphi'_{l,\lambda}(t_{\lambda,a}))/\sqrt{\lambda\varphi''_{l,\lambda}(t_{\lambda,a})}$. Then, we divide the integral into two parts

$$\int_{y \geq c_{l,\lambda}} e^{-u_{l,\lambda}y} dF_{l,\lambda}(y) = \int_{y \geq c_{l,\lambda}} e^{-u_{l,\lambda}y} d\mathcal{N}(y) + \int_{y \geq c_{l,\lambda}} e^{-u_{l,\lambda}y} d(F_{l,\lambda}(y) - \mathcal{N}(y)) =: J_{l,1} + J_{l,2}. \quad (6.40)$$

The latter is estimated by integration by parts as

$$\begin{aligned} |J_{l,2}| &= \left| e^{-u_{l,\lambda}c_{l,\lambda}} (F_{l,\lambda}(c_{l,\lambda}) - \mathcal{N}(c_{l,\lambda})) + \int_{y \geq c_{l,\lambda}} u_{l,\lambda} e^{-u_{l,\lambda}y} (F_{l,\lambda}(y) - \mathcal{N}(y)) dy \right| \\ &\leq \left| e^{b_{l,\lambda}} + \int_{y \geq c_{l,\lambda}} u_{l,\lambda} e^{-u_{l,\lambda}y} dy \right| \sup_y |F_{l,\lambda}(y) - \mathcal{N}(y)| = 2e^{b_{l,\lambda}} \mathcal{O}\left(\lambda^{-\frac{1}{2}}\right) \end{aligned} \quad (6.41)$$

by $-u_{l,\lambda}c_{l,\lambda} = b_{l,\lambda}$ and (6.24).

Step 3: In this step, we calculate the former part $J_{l,1}$. The former part $J_{l,1}$ is also calculated by using

integration by parts as follows:

$$\begin{aligned}
& J_{l,1} \\
&= \frac{1}{\sqrt{2\pi}} \int_{y \geq c_{l,\lambda}} e^{-u_{\lambda}y} e^{-\frac{y^2}{2}} dy \\
&= \frac{1}{\sqrt{2\pi}} \left[\frac{e^{-\frac{c_{l,\lambda}^2}{2}} e^{b_{l,\lambda}}}{u_{l,\lambda}} - \frac{1}{u_{l,\lambda}} \int_{y \geq c_{l,\lambda}} y e^{-u_{\lambda}y} e^{-\frac{y^2}{2}} dy \right] \\
&= \frac{1}{\sqrt{2\pi}} \left[\frac{e^{-\frac{c_{l,\lambda}^2}{2}} e^{b_{l,\lambda}}}{u_{l,\lambda}} - \frac{1}{u_{l,\lambda}} \left[\frac{c_{l,\lambda} e^{-\frac{c_{l,\lambda}^2}{2}} e^{b_{l,\lambda}}}{u_{l,\lambda}} - \frac{1}{u_{l,\lambda}} \int_{y \geq c_{l,\lambda}} (1-y^2) e^{-u_{\lambda}y} e^{-\frac{y^2}{2}} dy \right] \right]. \tag{6.42}
\end{aligned}$$

Since $t_{\lambda,a} = f(\nu + \lambda^{-\frac{1}{2}}a) \rightarrow 1$, we have $t_{\lambda,a} \geq 0$ for large enough λ , which yields $u_{l,\lambda} \geq 0$. Hence, we have

$$\left| \int_{y \geq c_{l,\lambda}} (1-y^2) e^{-u_{\lambda}y} e^{-\frac{y^2}{2}} dy \right| \leq e^{-u_{\lambda}c_{l,\lambda}} \int_{y \geq c_{l,\lambda}} |1-y^2| e^{-\frac{y^2}{2}} dy = \mathcal{O}(1) e^{b_{l,\lambda}} \tag{6.43}$$

because Gaussian integrals are finite. By substituting (6.31) and (6.32), the constant $c_{1,\lambda}$ is calculated as

$$\begin{aligned}
c_{1,\lambda} &= \lambda^{\frac{1}{2}} (\nu + \lambda^{-\frac{1}{2}}a - \varphi'_{1,\lambda}(t_{\lambda,a})) \varphi''_{1,\lambda}(t_{\lambda,a})^{-\frac{1}{2}} \\
&= [(\nu - \varphi'_{0,\lambda}(1)) \lambda^{\frac{1}{2}} + (1 - \varphi''_{0,\lambda}(1) f'(\nu)) a - \Lambda''_{\lambda}(1) f'(\nu) a + \mathcal{O}(\lambda^{-\frac{1}{2}}) + \mathcal{O}(\lambda^{-2} \|\mathbf{Q}_{\lambda}\|^2)] \\
&\quad \times \varphi''(1)^{-\frac{1}{2}} [1 + \varphi''(1)^{-1} \Lambda''_{\lambda}(1) + \mathcal{O}(\lambda^{-\frac{1}{2}}) + \mathcal{O}(\lambda^{-2} \|\mathbf{Q}_{\lambda}\|^2)]^{-\frac{1}{2}}. \tag{6.44}
\end{aligned}$$

Due to Lemma 6.2, the equation (6.44) implies

$$c_{1,\lambda} = o(1). \tag{6.45}$$

Similarly, we have

$$\begin{aligned}
c_{0,\lambda} &= [(\nu - \varphi'_{0,\lambda}(1)) \lambda^{\frac{1}{2}} + (1 - \varphi''_{0,\lambda}(1) f'(\nu)) a + \mathcal{O}(\lambda^{-\frac{1}{2}})] \varphi''(1)^{-\frac{1}{2}} [1 + \mathcal{O}(\lambda^{-\frac{1}{2}})]^{-\frac{1}{2}} \\
&= o(1) \tag{6.46}
\end{aligned}$$

from (6.18), (6.19), (6.33) and (6.34). Thus, evaluating (6.42) with (6.43), (6.45) and (6.46), we have

$$J_{l,1} = \frac{e^{-\frac{c_{l,\lambda}^2}{2}} e^{b_{l,\lambda}}}{\sqrt{2\pi} u_{l,\lambda}} \left[1 + \frac{1}{u_{l,\lambda}} \mathcal{O}(1) \right] = \frac{e^{-\frac{c_{l,\lambda}^2}{2}} e^{b_{l,\lambda}}}{\sqrt{2\pi} u_{l,\lambda}} \left[1 + \mathcal{O}(\lambda^{-\frac{1}{2}}) \right], \tag{6.47}$$

where we apply $u_{l,\lambda} = \mathcal{O}(\sqrt{\lambda})$ for the last equality.

Step 4: We make further calculation of $c_{i,\lambda}^2$. Squaring (6.44), we have

$$\begin{aligned}
c_{1,\lambda}^2 &= [(\nu - \varphi'_{0,\lambda}(1))^2 \lambda - 2(\nu - \varphi'_{0,\lambda}(1))\Lambda''_{\lambda}(1)f'(\nu)\lambda^{\frac{1}{2}}a + (1 - \varphi''_{0,\lambda}(1)f'(\nu))^2 a^2 + \Lambda''_{\lambda}(1)^2 f'(\nu)^2 a^2 \\
&\quad - 2(1 - \varphi''_{0,\lambda}(1)f'(\nu))f'(\nu)a^2 \Lambda''_{\lambda}(1) + 2(1 - \varphi''_{0,\lambda}(1)f'(\nu))(\nu - \varphi'_{0,\lambda}(1))\lambda^{\frac{1}{2}}a + \mathcal{O}(\lambda^{-\frac{1}{2}}) + \mathcal{O}(\lambda^{-2}\|\mathbf{Q}_{\lambda}\|^2)] \\
&\quad \times \varphi''(1)^{-1}[1 - \varphi''(1)^{-1}\Lambda''_{\lambda}(1) + \mathcal{O}(\lambda^{-\frac{1}{2}}) + \mathcal{O}(\lambda^{-2}\|\mathbf{Q}_{\lambda}\|^2)] \\
&\stackrel{(a)}{=} [(\nu - \varphi'_{0,\lambda}(1))^2 \lambda - 2(\nu - \varphi'_{0,\lambda}(1))\Lambda''_{\lambda}(1)f'(\nu)\lambda^{\frac{1}{2}}a + \mathcal{O}(\lambda^{-\frac{1}{2}}) + \mathcal{O}(\lambda^{-2}\|\mathbf{Q}_{\lambda}\|^2)] \\
&\quad \times \varphi''(1)^{-1}[1 - \varphi''(1)^{-1}\Lambda''_{\lambda}(1) + \mathcal{O}(\lambda^{-\frac{1}{2}}) + \mathcal{O}(\lambda^{-2}\|\mathbf{Q}_{\lambda}\|^2)] \\
&= \varphi''(1)^{-1}(\nu - \varphi'_{0,\lambda}(1))^2 \lambda - 2\varphi''(1)^{-1}(\nu - \varphi'_{0,\lambda}(1))\Lambda''_{\lambda}(1)f'(\nu)\lambda^{\frac{1}{2}}a \\
&\quad - \varphi''(1)^{-2}\Lambda''_{\lambda}(1)(\nu - \varphi'_{0,\lambda}(1))^2 \lambda + 2\varphi''(1)^{-2}(\nu - \varphi'_{0,\lambda}(1))\Lambda''_{\lambda}(1)^2 f'(\nu)\lambda^{\frac{1}{2}}a + \mathcal{O}(\lambda^{-\frac{1}{2}}) + \mathcal{O}(\lambda^{-2}\|\mathbf{Q}_{\lambda}\|^2) \\
&\stackrel{(b)}{=} \varphi''(1)^{-1}(\nu - \varphi'_{0,\lambda}(1))^2 \lambda - 2\varphi''(1)^{-1}(\nu - \varphi'_{0,\lambda}(1))\Lambda''_{\lambda}(1)f'(\nu)\lambda^{\frac{1}{2}}a \\
&\quad - \varphi''(1)^{-2}\Lambda''_{\lambda}(1)(\nu - \varphi'_{0,\lambda}(1))^2 \lambda + \mathcal{O}(\lambda^{-\frac{1}{2}}) + \mathcal{O}(\lambda^{-2}\|\mathbf{Q}_{\lambda}\|^2), \tag{6.48}
\end{aligned}$$

where the terms $\Lambda''_{\lambda}(1)^2 f'(\nu)^2 a^2$, $(1 - \varphi''_{0,\lambda}(1)f'(\nu))^2 a^2$, $2(1 - \varphi''_{0,\lambda}(1)f'(\nu))f'(\nu)a^2 \Lambda''_{\lambda}(1)$, and $2(1 - \varphi''_{0,\lambda}(1)f'(\nu))(\nu - \varphi'_{0,\lambda}(1))\lambda^{\frac{1}{2}}a$ are included in $\mathcal{O}(\lambda^{-\frac{1}{2}}) + \mathcal{O}(\lambda^{-2}\|\mathbf{Q}_{\lambda}\|^2)$ at (a) because of (6.18)-(6.20), and (b) follows from

$$(\nu - \varphi'_{0,\lambda}(1))\Lambda''_{\lambda}(1)^2 \lambda^{\frac{1}{2}} = \mathcal{O}(\lambda^{\alpha - \frac{1}{2}} \lambda^{-2} \|\mathbf{Q}_{\lambda}\|^2) = \mathcal{O}(\lambda^{-2} \|\mathbf{Q}_{\lambda}\|^2), \tag{6.49}$$

which is obtained from (6.18), (6.20) and $\alpha < \frac{1}{2}$. Similarly, we have

$$c_{0,\lambda}^2 = \varphi''(1)^{-1}(\nu - \varphi'_{0,\lambda}(1))^2 \lambda + \mathcal{O}(\lambda^{-\frac{1}{2}}) + \mathcal{O}(\lambda^{-2}\|\mathbf{Q}_{\lambda}\|^2). \tag{6.50}$$

Step 5: Finally, we calculate $N_1^{(\lambda)}(a)$. That is, we obtain

$$\begin{aligned}
\frac{1}{d_{\lambda}} N_1^{(\lambda)}(a) &= \mathbb{P}(Z_{1,\lambda} \geq \nu + \lambda^{-\frac{1}{2}}a) \\
&\stackrel{(a)}{=} e^{\lambda[\varphi_{1,\lambda}(t_{\lambda,a}) - t_{\lambda,a}(\nu + \lambda^{-\frac{1}{2}}a)]} e^{-b_{1,\lambda}} \frac{e^{-\frac{c_{1,\lambda}^2}{2}} e^{b_{1,\lambda}}}{\sqrt{2\pi u_{1,\lambda}}} \left[1 + \mathcal{O}(\lambda^{-\frac{1}{2}}) \right] \\
&\stackrel{(b)}{=} \frac{1}{d_{\lambda}} \exp \left[-\lambda\nu + [\varphi'_{0,\lambda}(1)f'(\nu) - \nu f'(\nu) - 1]\lambda^{\frac{1}{2}}a \right. \\
&\quad \left. + \left[\frac{1}{2}\varphi'_{0,\lambda}(1)f''(\nu) + \frac{1}{2}\varphi''_{0,\lambda}(1)f'(\nu)^2 - f'(\nu) - \frac{1}{2}\nu f''(\nu) + \frac{1}{2}\Lambda''_{\lambda}(1)f'(\nu)^2 + \mathcal{O}(\lambda^{\alpha-2}\|\mathbf{Q}_{\lambda}\|) \right] a^2 \right. \\
&\quad \left. - \frac{1}{2}c_{1,\lambda}^2 - \log \sqrt{2\pi} u_{1,\lambda} + \mathcal{O}(\lambda^{-\frac{1}{2}}) \right] \\
&\stackrel{(c)}{=} \frac{1}{d_{\lambda}} \exp \left[\left[\frac{1}{2}\varphi'_{0,\lambda}(1)f''(\nu) + \frac{1}{2}\varphi''_{0,\lambda}(1)f'(\nu)^2 - f'(\nu) - \frac{1}{2}\nu f''(\nu) + \frac{1}{2}\Lambda''_{\lambda}(1)f'(\nu)^2 \right] a^2 \right. \\
&\quad \left. + [\varphi'_{0,\lambda}(1)f'(\nu) - \nu f'(\nu) - 1 + \varphi''(1)^{-1}(\nu - \varphi'_{0,\lambda}(1))\Lambda''_{\lambda}(1)f'(\nu)]\lambda^{\frac{1}{2}}a \right. \\
&\quad \left. - \lambda\nu - \frac{1}{2}\varphi''(1)^{-1}(\nu - \varphi'_{0,\lambda}(1))^2 \lambda - \log \sqrt{2\pi} - \frac{1}{2} \log \varphi''(1) - \frac{1}{2} \log \lambda \right. \\
&\quad \left. + \frac{1}{2}\varphi''(1)^{-2}\Lambda''_{\lambda}(1)(\nu - \varphi'_{0,\lambda}(1))^2 \lambda - \frac{1}{2\varphi''(1)}\Lambda''_{\lambda}(1) + \mathcal{O}(\lambda^{-\frac{1}{2}}) + \mathcal{O}(\lambda^{-2}\|\mathbf{Q}_{\lambda}\|^2) \right], \tag{6.51}
\end{aligned}$$

where (a) follows from combining (6.41), (6.47) with (6.39), and we apply (6.29) and (6.30) to $\varphi_{1,\lambda}(t_{\lambda,a}) - t_{\lambda,a}(\nu + \lambda^{-\frac{1}{2}}a)$ at (b), and we substitute (6.35), (6.36), (6.48) and (6.50) at (c). Similarly, we have

$$\begin{aligned} \frac{1}{d_\lambda} N_0^{(\lambda)} &= \mathbb{P}(Z_{l,\lambda} \geq \nu + \lambda^{-\frac{1}{2}}a) \\ &= \frac{1}{d_\lambda} \exp \left[\left[\frac{1}{2} \varphi'_{0,\lambda}(1) f''(\nu) + \frac{1}{2} \varphi''_{0,\lambda}(1) f'(\nu)^2 - f'(\nu) - \frac{1}{2} \nu f''(\nu) \right] a^2 \right. \\ &\quad \left. + [\varphi'_{0,\lambda}(1) f'(\nu) - \nu f'(\nu) - 1] \lambda^{\frac{1}{2}} a \right. \\ &\quad \left. - \lambda \nu - \frac{1}{2} \varphi''(1)^{-1} (\nu - \varphi'_{0,\lambda}(1))^2 \lambda - \log \sqrt{2\pi} - \frac{1}{2} \log \varphi''(1) - \frac{1}{2} \log \lambda + \mathcal{O}(\lambda^{-\frac{1}{2}}) \right]. \end{aligned} \quad (6.52)$$

The equations (6.51) and (6.52) are equivalent with (6.14) and (6.15), hence the proof is completed. \square

7 Key Estimations for the proof of Theorems 4.1 and 4.2

In this section, we show the key estimations of the relative entropy (Lemma 7.1) and Fisher information (Lemma 7.2) needed for the proof of Theorems 4.1 and 4.2. We carry out all the proofs so that they are valid in the case where the observables $A_{i,\lambda}$, $B_{i,\lambda}$ are not necessarily commutative.

7.1 Estimation of the relative entropy by applying the strong large deviation

We implement the estimation of the relative entropy for the proof of Theorems 4.1 and 4.2 in the main text by using Lemma 6.1 prepared in the previous section. Our goal is the following lemma:

Lemma 7.1. *Under Assumption 4.1 and $\lambda^{\frac{5}{8}} \ll \|\mathbf{Q}_\lambda\| \ll \lambda$, we have*

$$\begin{aligned} D(\rho_{\text{opt}}^{(\lambda)} \| \tau_{\boldsymbol{\theta}_\lambda}^{(\lambda)}) &= \mathcal{O}\left(\frac{\|\mathbf{Q}_\lambda\|^2}{\lambda^2}\right) + \mathcal{O}\left(\lambda^{-\frac{1}{2}}\right) \\ D(\rho_{\text{opt,nc}}^{(\lambda)} \| \tau_{\boldsymbol{\theta}_\lambda}^{(\lambda)}) &= \mathcal{O}\left(\frac{\|\mathbf{Q}_\lambda\|^2}{\lambda^2}\right) + \mathcal{O}\left(\lambda^{-\frac{1}{2}}\right). \end{aligned} \quad (7.1)$$

Proof. We proceed the estimation as follows in a similar method to [19, 43]. At first, we deal with the case when $A_{i,\lambda}$, $B_{i,\lambda}$ ($i = 1, 2$) are mutually commutative. We stepwise reduce our problem as follows.

Step 1: From the construction of $\rho_{\text{opt}}^{(\lambda)}$, the following holds:

$$\begin{aligned} &D(\rho_{\text{opt}}^{(\lambda)} \| \tau_{\boldsymbol{\theta}_\lambda}^{(\lambda)}) \\ &= \text{tr} \rho_{\text{opt}}^{(\lambda)} (\log \rho_{\text{opt}}^{(\lambda)} - \log \tau_{\boldsymbol{\theta}_\lambda}^{(\lambda)}) \\ &= \sum_j p_{\boldsymbol{\theta}_0}^{(\lambda)}(j) (\log p_{\boldsymbol{\theta}_0}^{(\lambda)}(j) - \log p_{\boldsymbol{\theta}_\lambda}^{(\lambda)}(j)). \end{aligned} \quad (7.2)$$

Defining the random variable

$$Y_l^{(\lambda)}(j) := \begin{cases} \frac{\log p_{\boldsymbol{\theta}_0}^{(\lambda)}(j) - \lambda \nu}{\sqrt{\lambda}} & (l = 0) \\ \frac{\log p_{\boldsymbol{\theta}_\lambda}^{(\lambda)}(j) - \lambda \nu}{\sqrt{\lambda}} & (l = 1), \end{cases} \quad (7.3)$$

we have another expression the relative entropy

$$D(\rho_{\text{opt}}^{(\lambda)} \parallel \tau_{\theta_\lambda}^{(\lambda)}) = \sqrt{\lambda} \left(\mathbb{E}_{p_{\theta_0}^{(\lambda)}}[Y_0^{(\lambda)}] - \mathbb{E}_{p_{\theta_0}^{(\lambda)}}[Y_1^{(\lambda)}] \right), \quad (7.4)$$

where $\mathbb{E}_p[X]$ denotes the expectation value of a random variable X with probability distribution p . To estimate the relative entropy, it is difficult to calculate $\mathbb{E}_{p_{\theta_0}^{(\lambda)}}[Y_1^{(\lambda)}]$. Instead, we approximate $\Delta_\lambda(j) := Y_0^{(\lambda)}(j) - Y_1^{(\lambda)}(j)$ by a quadratic polynomial of $Y_0^{(\lambda)}(j)$. In this way, we can calculate $\mathbb{E}_{p_{\theta_0}^{(\lambda)}}[\Delta_\lambda]$ by calculating the moments of $Y_0^{(\lambda)}$.

Step 2: To compare $Y_1^{(\lambda)}(j)$ with $Y_0^{(\lambda)}(j)$, we compare the number of states $N_1^{(\lambda)}$ with $N_0^{(\lambda)}$ defined by (6.1). The number of states $N_l^{(\lambda)}$ is expressed by $Y_l^{(\lambda)}$ as

$$N_l^{(\lambda)}(a) = \left| \left\{ j \mid Y_l^{(\lambda)}(j) \geq a \right\} \right|. \quad (7.5)$$

As will be shown in **Step 3**, the equation

$$\log N_1^{(\lambda)}(a - x) = \log N_0^{(\lambda)}(a) \quad (7.6)$$

for x with a constant a is asymptotically solved as

$$\begin{aligned} \sqrt{\lambda}x &= -\frac{1}{2}\Lambda_\lambda''(1)f'(\nu)^2a^2 - \varphi''(1)^{-1}(\nu - \varphi'_{0,\lambda}(1))\Lambda_\lambda''(1)f'(\nu)\lambda^{\frac{1}{2}}a \\ &\quad - \frac{1}{2}\varphi''(1)^{-2}\Lambda_\lambda''(1)(\nu - \varphi'_{0,\lambda}(1))^2\lambda + \frac{1}{2\varphi''(1)}\Lambda_\lambda''(1) + \mathcal{O}\left(\lambda^{-\frac{1}{2}}\right) + \mathcal{O}(\lambda^{-2}\|\mathbf{Q}_\lambda\|^2) \\ &=: \sqrt{\lambda}q_\lambda(a) + \mathcal{O}\left(\lambda^{-\frac{1}{2}}\right) + \mathcal{O}(\lambda^{-2}\|\mathbf{Q}_\lambda\|^2), \end{aligned} \quad (7.7)$$

Since $Y_l^{(\lambda)}$ satisfies

$$Y_l^{(\lambda)}(1) \geq Y_l^{(\lambda)}(2) \geq Y_l^{(\lambda)}(3) \geq \dots \quad (7.8)$$

by its definition, $\log N_l^{(\lambda)}(Y_l^{(\lambda)}(j))$ is asymptotically equal to $\log j$. Thus, the equation

$$\log N_1^{(\lambda)}(Y_1^{(\lambda)}(j)) = \log N_0^{(\lambda)}(Y_0^{(\lambda)}(j)) \quad (7.9)$$

holds asymptotically. Thus, $\Delta_\lambda(j) = Y_0^{(\lambda)}(j) - Y_1^{(\lambda)}(j)$ satisfies

$$\log N_1^{(\lambda)}(Y_0^{(\lambda)}(j) - \Delta_\lambda(j)) = \log N_0^{(\lambda)}(Y_0^{(\lambda)}(j)). \quad (7.10)$$

Then, we obtain the approximation of $\Delta_\lambda(j)$ by the solution (7.7) of the equation (7.6) as

$$\begin{aligned} &\sqrt{\lambda}\Delta_\lambda(j) \\ &= \sqrt{\lambda}q_\lambda(Y_0^{(\lambda)}(j)) + \mathcal{O}\left(\lambda^{-\frac{1}{2}}\right) + \mathcal{O}(\lambda^{-2}\|\mathbf{Q}_\lambda\|^2) \\ &= -\frac{1}{2}\Lambda_\lambda''(1)f'(\nu)^2(Y_0^{(\lambda)}(j))^2 \\ &\quad - \varphi''(1)^{-1}(\nu - \varphi'_{0,\lambda}(1))\Lambda_\lambda''(1)f'(\nu)\lambda^{\frac{1}{2}}Y_0^{(\lambda)}(j) \\ &\quad - \frac{1}{2}\varphi''(1)^{-2}\Lambda_\lambda''(1)(\nu - \varphi'_{0,\lambda}(1))^2\lambda + \frac{1}{2\varphi''(1)}\Lambda_\lambda''(1) + \mathcal{O}\left(\lambda^{-\frac{1}{2}}\right) + \mathcal{O}(\lambda^{-2}\|\mathbf{Q}_\lambda\|^2). \end{aligned} \quad (7.11)$$

Step 3: In this step, we show that the solution of the equation (7.6) is asymptotically given by (7.7). From the asymptotic expansions (6.14) and (6.15) in Lemma 6.1, the equation (7.6) is written as

$$r_{2,\lambda}^1(a-x)^2 + r_{1,\lambda}^1(a-x) + r_{0,\lambda}^1 + \mathcal{O}\left(\lambda^{-\frac{1}{2}}\right) + \mathcal{O}(\lambda^{-2}\|\mathbf{Q}_\lambda\|^2) = r_{2,\lambda}^0 a^2 + r_{1,\lambda}^0 a + r_{0,\lambda}^0 + \mathcal{O}\left(\lambda^{-\frac{1}{2}}\right), \quad (7.12)$$

which may be deformed as

$$r_{2,\lambda}^1 x^2 + (-2r_{2,\lambda}^1 a - r_{1,\lambda}^1)x - (r_{2,\lambda}^0 - r_{2,\lambda}^1)a^2 - (r_{1,\lambda}^0 - r_{1,\lambda}^1)a - r_{0,\lambda}^0 - r_{0,\lambda}^1 + \mathcal{O}\left(\lambda^{-\frac{1}{2}}\right) + \mathcal{O}(\lambda^{-2}\|\mathbf{Q}_\lambda\|^2) = 0. \quad (7.13)$$

Dividing the both sides of (7.13) by λ and changing the variable x to $y := x/\sqrt{\lambda}$, we have the equation for y as

$$q_{2,\lambda}y^2 + q_{1,\lambda}y + \epsilon_\lambda = 0, \quad (7.14)$$

where

$$q_{2,\lambda} := r_{2,\lambda}^1 = \mathcal{O}(1) \quad (7.15)$$

$$q_{1,\lambda} := -r_{1,\lambda}^1 \lambda^{-\frac{1}{2}} + \mathcal{O}\left(\lambda^{-\frac{1}{2}}\right) = \mathcal{O}(1) \quad (7.16)$$

$$\epsilon_\lambda := \lambda^{-1}[-(r_{2,\lambda}^0 - r_{2,\lambda}^1)a^2 - (r_{1,\lambda}^0 - r_{1,\lambda}^1)a - r_{0,\lambda}^0 - r_{0,\lambda}^1 + \mathcal{O}\left(\lambda^{-\frac{1}{2}}\right) + \mathcal{O}(\lambda^{-2}\|\mathbf{Q}_\lambda\|^2)] = \mathcal{O}(\lambda^{-2}\|\mathbf{Q}_\lambda\|). \quad (7.17)$$

The perturbation from $y = 0$ up to $\mathcal{O}(\epsilon_\lambda)$ gives

$$y = -\frac{\epsilon_\lambda}{q_{1,\lambda}} + \mathcal{O}(\epsilon_\lambda^2) = -\frac{\epsilon_\lambda}{q_{1,\lambda}} + \mathcal{O}(\lambda^{-4}\|\mathbf{Q}_\lambda\|^2). \quad (7.18)$$

In fact, substituting it to the left hand side of (7.14), we have

$$q_{2,\lambda}y^2 + q_{1,\lambda}y + \epsilon_\lambda = \mathcal{O}(\epsilon_\lambda^2) - \epsilon_\lambda + \epsilon_\lambda = \mathcal{O}(\epsilon_\lambda^2). \quad (7.19)$$

Therefore, we obtain

$$\begin{aligned} \sqrt{\lambda}x = \lambda y &= -\lambda \frac{\epsilon_\lambda}{q_{1,\lambda}} + \mathcal{O}(\lambda^{-3}\|\mathbf{Q}_\lambda\|^2) \\ &= -\frac{\sqrt{\lambda}}{r_{1,\lambda}^1}[(r_{2,\lambda}^0 - r_{2,\lambda}^1)a^2 + (r_{1,\lambda}^0 - r_{1,\lambda}^1)a + r_{0,\lambda}^0 - r_{0,\lambda}^1] + \mathcal{O}\left(\lambda^{-\frac{1}{2}}\right) + \mathcal{O}(\lambda^{-2}\|\mathbf{Q}_\lambda\|^2). \end{aligned} \quad (7.20)$$

Thus, substituting $r_{t,\lambda}^{(j)}$ given by (6.8)-(6.13) in Lemma 6.1 to (7.20), we have

$$\begin{aligned}
\sqrt{\lambda}x &= [1 - (\varphi'_{0,\lambda}(1) - \nu)f'(\nu) - \varphi''(1)^{-1}(\nu - \varphi'_{0,\lambda}(1))\Lambda''_{\lambda}(1)f'(\nu)]^{-1} \\
&\quad \times \left[-\frac{1}{2}\Lambda''_{\lambda}(1)f'(\nu)^2a^2 - \varphi''(1)^{-1}(\nu - \varphi'_{0,\lambda}(1))\Lambda''_{\lambda}(1)f'(\nu)\lambda^{\frac{1}{2}}a \right. \\
&\quad \left. - \frac{1}{2}\varphi''(1)^{-2}\Lambda''_{\lambda}(1)(\nu - \varphi'_{0,\lambda}(1))^2\lambda + \frac{1}{2\varphi''(1)}\Lambda''_{\lambda}(1) \right] + \mathcal{O}(\lambda^{-\frac{1}{2}}) + \mathcal{O}(\lambda^{-2}\|\mathbf{Q}_{\lambda}\|^2) \\
&\stackrel{(a)}{=} \left[1 + \mathcal{O}(\lambda^{-\frac{1}{2}}) \right] \\
&\quad \times \left[-\frac{1}{2}\Lambda''_{\lambda}(1)f'(\nu)^2a^2 - \varphi''(1)^{-1}(\nu - \varphi'_{0,\lambda}(1))\Lambda''_{\lambda}(1)f'(\nu)\lambda^{\frac{1}{2}}a \right. \\
&\quad \left. - \frac{1}{2}\varphi''(1)^{-2}\Lambda''_{\lambda}(1)(\nu - \varphi'_{0,\lambda}(1))^2\lambda + \frac{1}{2\varphi''(1)}\Lambda''_{\lambda}(1) \right] + \mathcal{O}(\lambda^{-\frac{1}{2}}) + \mathcal{O}(\lambda^{-2}\|\mathbf{Q}_{\lambda}\|^2) \\
&= -\frac{1}{2}\Lambda''_{\lambda}(1)f'(\nu)^2a^2 - \varphi''(1)^{-1}(\nu - \varphi'_{0,\lambda}(1))\Lambda''_{\lambda}(1)f'(\nu)\lambda^{\frac{1}{2}}a \\
&\quad - \frac{1}{2}\varphi''(1)^{-2}\Lambda''_{\lambda}(1)(\nu - \varphi'_{0,\lambda}(1))^2\lambda + \frac{1}{2\varphi''(1)}\Lambda''_{\lambda}(1) + \mathcal{O}(\lambda^{-\frac{1}{2}}) + \mathcal{O}(\lambda^{-2}\|\mathbf{Q}_{\lambda}\|^2),
\end{aligned}$$

where (a) is verified by observing that $(\varphi'_{0,\lambda}(1) - \nu)f'(\nu)$ and $\varphi''(1)^{-1}(\nu - \varphi'_{0,\lambda}(1))\Lambda''_{\lambda}(1)f'(\nu)$ are included in $+\mathcal{O}(\lambda^{-\frac{1}{2}}) + \mathcal{O}(\lambda^{-2}\|\mathbf{Q}_{\lambda}\|^2)]^{-\frac{1}{2}}$ because of Lemma 6.2.

Step 4: Finally, in this step, we evaluate the relative entropy $D(\rho_{\text{opt}}^{(\lambda)}\|\tau_{\theta_{\lambda}}^{(\lambda)})$ by using (7.11). Because

$$\begin{aligned}
\varphi''_{0,\lambda}(1) &= \lambda^{-1} \sum_{i,j} \frac{\partial^2 \phi_{\lambda}}{\partial \theta^i \partial \theta^j}(\boldsymbol{\theta}_0) \theta_0^i \theta_0^j \\
&= \lambda^{-1} \text{tr} \left[\tau_{\boldsymbol{\theta}_0}^{(\lambda)} \sum_i \theta_0^i (X_{i,\lambda} - \eta_{\lambda,i}(\boldsymbol{\theta}_0)) \sum_j \theta_0^j (X_{j,\lambda} - \eta_{\lambda,j}(\boldsymbol{\theta}_0)) \right] \\
&= \lambda^{-1} \text{tr} \tau_{\boldsymbol{\theta}_0}^{(\lambda)} (-\log \tau_{\boldsymbol{\theta}_0}^{(\lambda)} - S(\tau_{\boldsymbol{\theta}_0}^{(\lambda)}))^2 \\
&= \lambda^{-1} \mathbb{E}_{p_{\boldsymbol{\theta}_0}^{(\lambda)}} [(-\log p_{\boldsymbol{\theta}_0}^{(\lambda)} - S(\tau_{\boldsymbol{\theta}_0}^{(\lambda)}))^2]
\end{aligned} \tag{7.21}$$

holds, we have

$$\mathbb{E}_{p_{\boldsymbol{\theta}_0}^{(\lambda)}} [Y_0^{(\lambda)}] = -\sqrt{\lambda}(\nu - \varphi'_{0,\lambda}(1)), \tag{7.22}$$

$$\begin{aligned}
\mathbb{E}_{p_{\boldsymbol{\theta}_0}^{(\lambda)}} [(Y_0^{(\lambda)})^2] &= \lambda^{-1} \mathbb{E}_{p_{\boldsymbol{\theta}_0}^{(\lambda)}} [(-\log p_{\boldsymbol{\theta}_0}^{(\lambda)} - S(\tau_{\boldsymbol{\theta}_0}^{(\lambda)}))^2] + (S(\tau_{\boldsymbol{\theta}_0}^{(\lambda)}) - \lambda\nu)^2 \\
&= \varphi''_{0,\lambda}(1) + \lambda(\nu - \varphi'_{0,\lambda}(1))^2 + \mathcal{O}(\lambda^{-\frac{1}{2}}) \\
&= \varphi''(1) + \lambda(\nu - \varphi'_{0,\lambda}(1))^2 + \mathcal{O}(\lambda^{-\frac{1}{2}}),
\end{aligned} \tag{7.23}$$

$$f'(\nu) = \frac{1}{\varphi''(1)} \tag{7.24}$$

in view of (6.6). Thus, we obtain

$$\begin{aligned}
& D(\rho_{\text{opt}}^{(\lambda)} \parallel \tau_{\theta_\lambda}^{(\lambda)}) \\
& \stackrel{(a)}{=} \sqrt{\lambda} \mathbb{E}_{p_{\theta_0}^{(\lambda)}}[\Delta_\lambda] \\
& \stackrel{(b)}{=} -\frac{1}{2} \Lambda_\lambda''(1) f'(\nu)^2 \mathbb{E}_{p_{\theta_0}^{(\lambda)}}[(Y_0^{(\lambda)})^2] \\
& \quad - \varphi''(1)^{-1} (\nu - \varphi'_{0,\lambda}(1)) \Lambda_\lambda''(1) f'(\nu) \lambda^{\frac{1}{2}} \mathbb{E}_{p_{\theta_0}^{(\lambda)}}[Y_0^{(\lambda)}] \\
& \quad - \frac{1}{2} \varphi''(1)^{-2} \Lambda_\lambda''(1) (\nu - \varphi'_{0,\lambda}(1))^2 \lambda + \frac{1}{2\varphi''(1)} \Lambda_\lambda''(1) + \mathcal{O}(\lambda^{-\frac{1}{2}}) + \mathcal{O}(\lambda^{-2} \|\mathbf{Q}_\lambda\|^2) \\
& \stackrel{(c)}{=} -\frac{1}{2\varphi''(1)} \Lambda_\lambda''(1) + \frac{1}{2\varphi''(1)} \Lambda_\lambda''(1) \\
& \quad + \varphi''(1)^{-2} \Lambda_\lambda''(1) (\nu - \varphi'_{0,\lambda}(1))^2 \lambda - \frac{1}{2} \varphi''(1)^{-2} \Lambda_\lambda''(1) (\nu - \varphi'_{0,\lambda}(1))^2 \lambda - \frac{1}{2} \varphi''(1)^{-2} \Lambda_\lambda''(1) (\nu - \varphi'_{0,\lambda}(1))^2 \lambda \\
& \quad + \mathcal{O}(\lambda^{-\frac{1}{2}}) + \mathcal{O}(\lambda^{-2} \|\mathbf{Q}_\lambda\|^2) \\
& = \mathcal{O}(\lambda^{-\frac{1}{2}}) + \mathcal{O}(\lambda^{-2} \|\mathbf{Q}_\lambda\|^2), \tag{7.25}
\end{aligned}$$

where (a) and (b) follow from (7.4) and (7.11) respectively, and (c) follows from substituting (7.22)-(7.24). Hence, we obtain the desired estimation for $D(\rho_{\text{opt}}^{(\lambda)} \parallel \tau_{\theta_\lambda}^{(\lambda)})$.

Non-commutative case: For non-commutative $A_{i,\lambda}$ and $B_{i,\lambda}$ ($i = 1, 2$), since $\rho_{\text{opt,nc}}^{(\lambda)}$ commutes with $\tau_{\theta_\lambda}^{(\lambda)}$ by its construction, we also have

$$\begin{aligned}
& D(\rho_{\text{opt,nc}}^{(\lambda)} \parallel \tau_{\theta_\lambda}^{(\lambda)}) \\
& = \text{tr} \rho_{\text{opt,nc}}^{(\lambda)} (\log \rho_{\text{opt,nc}}^{(\lambda)} - \log \tau_{\theta_\lambda}^{(\lambda)}) \\
& = \sum_j p_{\theta_0}^{(\lambda)}(j) (\log p_{\theta_0}^{(\lambda)}(j) - \log p_{\theta_\lambda}^{(\lambda)}(j)). \tag{7.26}
\end{aligned}$$

Thus, we can define $Y_l^{(\lambda)}(j)$ as with (7.3). Therefore, Step 1 and Step 2 are completely the same as the commutative case because it is sufficient to deal with just the probability distributions composed of the eigenvalue of the thermal states. In Step 3, (7.22) also holds for the non-commutative case. In addition,

(7.23) is also valid because we have

$$\begin{aligned}
\varphi''_{0,\lambda}(1) &= \lambda^{-1} \sum_{i,j} \frac{\partial^2 \phi_\lambda}{\partial \theta^i \partial \theta^j}(\boldsymbol{\theta}_0) \theta_0^i \theta_0^j \\
&= \lambda^{-1} \sum_{i,j} \int_0^1 ds \operatorname{tr} \left[\left(\tau_{\boldsymbol{\theta}_0}^{(\lambda)} \right)^{1-s} (X_{i,\lambda} - \eta_{\lambda,i}(\boldsymbol{\theta}_0)) \left(\tau_{\boldsymbol{\theta}_0}^{(\lambda)} \right)^s (X_{j,\lambda} - \eta_{\lambda,j}(\boldsymbol{\theta}_0)) \right] \theta_0^i \theta_0^j \\
&= \lambda^{-1} \int_0^1 ds \operatorname{tr} \left[\left(\tau_{\boldsymbol{\theta}_0}^{(\lambda)} \right)^{1-s} \sum_i \theta_0^i (X_{i,\lambda} - \eta_{\lambda,i}(\boldsymbol{\theta}_0)) \left(\tau_{\boldsymbol{\theta}_0}^{(\lambda)} \right)^s \sum_j \theta_0^j (X_{j,\lambda} - \eta_{\lambda,j}(\boldsymbol{\theta}_0)) \right] \\
&\stackrel{(a)}{=} \lambda^{-1} \operatorname{tr} \left[\tau_{\boldsymbol{\theta}_0}^{(\lambda)} \sum_i \theta_0^i (X_{i,\lambda} - \eta_{\lambda,i}(\boldsymbol{\theta}_0)) \sum_j \theta_0^j (X_{j,\lambda} - \eta_{\lambda,j}(\boldsymbol{\theta}_0)) \right] \\
&= \lambda^{-1} \operatorname{tr} \tau_{\boldsymbol{\theta}_0}^{(\lambda)} (-\log \tau_{\boldsymbol{\theta}_0}^{(\lambda)} - S(\tau_{\boldsymbol{\theta}_0}^{(\lambda)}))^2 \\
&= \lambda^{-1} \mathbb{E}_{p_{\boldsymbol{\theta}_0}^{(\lambda)}} [(-\log p_{\boldsymbol{\theta}_0}^{(\lambda)} - S(\tau_{\boldsymbol{\theta}_0}^{(\lambda)}))^2], \tag{7.27}
\end{aligned}$$

where (a) follows from that $\tau_{\boldsymbol{\theta}_0}^{(\lambda)} = \exp[\sum_i \theta_0^i X_{i,\lambda} - \phi_\lambda(\boldsymbol{\theta}_0)]$ commutes with $\sum_i \theta_0^i X_{i,\lambda}$. Thus, Step 3 is also the same as the commutative case. Then, the proof is completed. \square

7.2 Estimation of the Fisher information

Next, we deal with the estimation of the Fisher information $\max_{t \in [0,1]} \|(J_{\lambda,ij}(\mathbf{s}_\lambda(t)))_{ij}\|$ in Sec. 4.4. Recall that $\mathbf{s}_\lambda(t)$ is defined as the generalized inverse temperature such that

$$\boldsymbol{\eta}_\lambda(\mathbf{s}_\lambda(t)) = t\boldsymbol{\eta}_\lambda(\boldsymbol{\theta}_\lambda) + (1-t)\boldsymbol{\eta}_\lambda(\boldsymbol{\xi}_\lambda) \tag{7.28}$$

by the ideal inverse temperature $\boldsymbol{\theta}_\lambda$ associated with a vector \mathbf{Q}_λ , and the effective inverse temperature $\boldsymbol{\xi}_\lambda := \tilde{\boldsymbol{\theta}}_\lambda(\rho_{\text{opt},(\text{nc})}^{(\lambda)})$ of the final state $\rho_{\text{opt}}^{(\lambda)}$ ($\rho_{\text{opt},(\text{nc})}^{(\lambda)}$) of our protocol (for the non-commutative case). We show the following estimation of the Fisher information $J_{\lambda,ij}$ defined by (2.4):

Lemma 7.2. *Under Assumption 4.1 and $\lambda^{\frac{5}{8}} \ll \|\mathbf{Q}_\lambda\| \ll \lambda$, we have*

$$\max_{t \in [0,1]} \|(J_{\lambda,ij}(\mathbf{s}_\lambda(t)))_{ij}\| = \mathcal{O}(\lambda). \tag{7.29}$$

Proof. We consider for the non-commutative case, which of course includes the commutative case. First of all, since $\|A\| \leq \|A\|_1$ holds for any matrix A , where $\|A\|_1 = \operatorname{tr} |A|$ is the trace norm, we have

$$\begin{aligned}
\|(J_{\lambda,ij}(\mathbf{s}_\lambda(t)))_{ij}\| &\leq \operatorname{tr}(J_{\lambda,ij}(\mathbf{s}_\lambda(t)))_{ij} \\
&= \sum_{i=1}^4 \int_0^1 ds \operatorname{tr}(X_{i,\lambda} - \eta_{\lambda,i}(\mathbf{s}_\lambda(t))) \left(\tau_{\mathbf{s}_\lambda(t)}^{(\lambda)} \right)^s (X_{i,\lambda} - \eta_{\lambda,i}(\mathbf{s}_\lambda(t))) \left(\tau_{\mathbf{s}_\lambda(t)}^{(\lambda)} \right)^{1-s}, \tag{7.30}
\end{aligned}$$

where $X_{i,\lambda} = A_{i,\lambda}$, $X_{i+2,\lambda} = B_{i,\lambda}$ ($i = 1, 2$). Furthermore, for any $0 \leq s \leq 1$ we have

$$\operatorname{tr}(X_{i,\lambda} - \eta_{\lambda,i}(\mathbf{s}_\lambda(t))) \left(\tau_{\mathbf{s}_\lambda(t)}^{(\lambda)} \right)^s (X_{i,\lambda} - \eta_{\lambda,i}(\mathbf{s}_\lambda(t))) \left(\tau_{\mathbf{s}_\lambda(t)}^{(\lambda)} \right)^{1-s} \leq \operatorname{tr}(X_{i,\lambda} - \eta_{\lambda,i}(\mathbf{s}_\lambda(t)))^2 \tau_{\mathbf{s}_\lambda(t)}^{(\lambda)} \tag{7.31}$$

since the Wigner-Yanase-Dyson skew information [44–46]

$$I_{\rho,s}(X) := \text{tr } X^2 \rho - \text{tr } X \rho^s X \rho^{1-s} \quad (7.32)$$

is positive $I_{\rho,s}(X) \geq 0$ for any state ρ , observable X , and $0 \leq s \leq 1$. The positivity follows from the fact that $I_{\rho,s}(X)$ is convex with respect to ρ [47], because $I_{|\psi\rangle\langle\psi|,s}(X)$ is obviously positive for any pure state $|\psi\rangle$. Observing that

$$\text{tr}(X_{i,\lambda} - \eta_{\lambda,i}(\mathbf{s}_\lambda(t)))^2 \tau_{\mathbf{s}_\lambda(t)}^{(\lambda)} = \text{tr } X_{i,\lambda}^2 \tau_{\mathbf{s}_\lambda(t)}^{(\lambda)} - \eta_{\lambda,i}(\mathbf{s}_\lambda(t))^2 \leq \text{tr } X_{i,\lambda}^2 \tau_{\mathbf{s}_\lambda(t)}^{(\lambda)}, \quad (7.33)$$

The combination of (7.30) and (7.31) yields that

$$\|(J_{\lambda,ij}(\mathbf{s}_\lambda(t)))_{ij}\| \leq \sum_{i=1}^4 \text{tr } X_{i,\lambda}^2 \tau_{\mathbf{s}_\lambda(t)}^{(\lambda)}. \quad (7.34)$$

From the inequalities $\|AB\|_1 \leq \|A\| \|B\|_1$ and $\|A^2\| \leq \|A\|^2$ for any matrices A, B , and the assumption $\|X_{i,\lambda}\| = \mathcal{O}(\lambda)$, we obtain

$$\text{tr } X_{i,\lambda}^2 \tau_{\mathbf{s}_\lambda(t)}^{(\lambda)} \leq \|X_{i,\lambda}^2 \tau_{\mathbf{s}_\lambda(t)}^{(\lambda)}\|_1 \leq \|X_{i,\lambda}\|^2 \|\tau_{\mathbf{s}_\lambda(t)}^{(\lambda)}\|_1 \leq \|X_{i,\lambda}\|^2 = \mathcal{O}(\lambda^2) \quad (7.35)$$

since $\|\tau_{\mathbf{s}_\lambda(t)}^{(\lambda)}\|_1 = \text{tr } \tau_{\mathbf{s}_\lambda(t)}^{(\lambda)} = 1$. Thus, the combination of (7.34) and (7.35) implies that

$$\max_{t \in [0,1]} \|(J_{\lambda,ij}(\mathbf{s}_\lambda(t)))_{ij}\| = \mathcal{O}(\lambda^2). \quad (7.36)$$

Furthermore, we improve this estimation by using (4.25). Combining (7.36) and (4.25), we have

$$\begin{aligned} & \|\boldsymbol{\eta}_\lambda(\boldsymbol{\theta}_\lambda) - \boldsymbol{\eta}_\lambda(\boldsymbol{\xi}_\lambda)\| \\ &= \mathcal{O}\left(\sqrt{D(\rho_{\text{opt,nc}}^{(\lambda)} \|\tau_{\boldsymbol{\theta}_\lambda}^{(\lambda)}\|) \max_{t \in [0,1]} \|(J_{\lambda,ij}(\mathbf{s}_\lambda(t)))_{ij}\|}\right) \\ &= \mathcal{O}\left(D(\rho_{\text{opt,nc}}^{(\lambda)} \|\tau_{\boldsymbol{\theta}_\lambda}^{(\lambda)}\|)^{\frac{1}{2}} \lambda\right). \end{aligned} \quad (7.37)$$

Since we assumed $\|\mathbf{Q}_\lambda\| = o(\lambda)$, the relation $D(\rho_{\text{opt,nc}}^{(\lambda)} \|\tau_{\boldsymbol{\theta}_\lambda}^{(\lambda)}\|) = o(1)$ follows from Lemma 7.1, which implies $\|\boldsymbol{\eta}_\lambda(\boldsymbol{\theta}_0) - \boldsymbol{\eta}_\lambda(\boldsymbol{\xi}_\lambda)\| = o(\lambda)$ because of $\|\boldsymbol{\eta}_\lambda(\boldsymbol{\theta}_0) - \boldsymbol{\eta}_\lambda(\boldsymbol{\theta}_\lambda)\| = o(\lambda)$. Hence, the relation $\|\boldsymbol{\eta}_\lambda(\boldsymbol{\theta}_0) - \boldsymbol{\eta}_\lambda(\mathbf{s}_\lambda(t))\| = o(\lambda)$ holds for any $t \in [0, 1]$ since $\boldsymbol{\eta}_\lambda(\mathbf{s}_\lambda(t))$ is a convex combination of $\boldsymbol{\eta}_\lambda(\boldsymbol{\theta}_\lambda)$ and $\boldsymbol{\eta}_\lambda(\boldsymbol{\xi}_\lambda)$. Therefore,

$$\mathbf{s}_\lambda(t) \rightarrow \boldsymbol{\theta}_0 \quad (7.38)$$

holds. Because (2.8) and (7.38) imply that

$$J_{\lambda,ij}(\mathbf{s}_\lambda(t)) = \lambda g_{ij}(\boldsymbol{\theta}_0) + o(\lambda), \quad (7.39)$$

we have

$$\max_{t \in [0,1]} \|(J_{\lambda,ij}(\mathbf{s}_\lambda(t)))_{ij}\| = \mathcal{O}(\lambda). \quad (7.40)$$

□

8 Proofs of Theorems 4.1 and 4.2

Proof of Theorem 4.1. According to Lemma 7.1 in Sec. 7.1, the order $\lambda^{\frac{5}{8}} \ll \|\mathbf{Q}_\lambda\| \ll \lambda$ of the generalized heat is sufficient for

$$D(\rho_{\text{opt}}^{(\lambda)} \|\tau_{\theta_\lambda}^{(\lambda)}) = \mathcal{O}\left(\frac{\|\mathbf{Q}_\lambda\|^2}{\lambda^2}\right) + \mathcal{O}\left(\lambda^{-\frac{1}{2}}\right) \quad (8.1)$$

and

$$\max_{t \in [0,1]} \|(J_{\lambda,ij}(\mathbf{s}_\lambda(t)))_{ij}\| = \mathcal{O}(\lambda) \quad (8.2)$$

to be true. Thus, combining Lemma 4.1 and the above estimations, we have

$$\|\boldsymbol{\eta}_\lambda(\boldsymbol{\theta}_\lambda) - \boldsymbol{\eta}_\lambda(\boldsymbol{\xi}_\lambda)\| = \sqrt{\mathcal{O}\left(\frac{\|\mathbf{Q}_\lambda\|^2}{\lambda}\right) + \mathcal{O}\left(\lambda^{\frac{1}{2}}\right)}. \quad (8.3)$$

Finally, the order $\lambda^{\frac{5}{8}} \ll \|\mathbf{Q}_\lambda\|$ is sufficient for the right hand side (RHS) of (8.3) to be $o\left(\frac{\|\mathbf{Q}_\lambda\|^2}{\lambda}\right)$, i.e.

$$\|\boldsymbol{\eta}_\lambda(\boldsymbol{\theta}_\lambda) - \boldsymbol{\eta}_\lambda(\boldsymbol{\xi}_\lambda)\| = \sqrt{\mathcal{O}\left(\frac{\|\mathbf{Q}_\lambda\|^2}{\lambda}\right) + \mathcal{O}\left(\lambda^{\frac{1}{2}}\right)} = o\left(\frac{\|\mathbf{Q}_\lambda\|^2}{\lambda}\right). \quad (8.4)$$

Hence, Theorem 4.1 is proved. \square

Proof of Theorem 4.2. To show Theorem 4.2, it is enough to do the same process as above. At first, Lemma 4.1 holds by replacing $\rho_{\text{opt}}^{(\lambda)}$ with $\rho_{\text{opt,nc}}^{(\lambda)}$. The proof is the same since the Pythagorean theorem Lemma A.3 is proved with non-commutative observables in Appendix A.2, so that (4.26) holds. Furthermore, the estimations of the relative entropy (Lemma 7.1) and Fisher information (7.2) also hold for the non-commutative case. The remaining part obviously has nothing to do with non-commutativity. Thus, FGCB is also achieved in the non-commutative case in the semi-explicit battery formulation. \square

9 Examples

In this section, we give some examples of generalized heat engines to apply our general theory established in the above. In each case, we firstly have to verify the asymptotic extensivity (Assumption 2.1) to ensure the applicability of our setup. Then, we calculate the second order coefficients of the optimal performance to investigate the behavior of the finite-size effect for each model.

9.1 An ordinary heat engine with i.i.d. particles

As a first example, we verify that the model of the heat engine in the previous work [19] is included in our theory. In this heat engine, the hot and the cold baths consist of n particles with Hamiltonian H_h and H_c respectively. Quantity A is the energy, and Quantity B is empty in this case. The scale parameter is the number n of the particles. The scale dependent observables of the hot and the cold baths are $H_{h,n} := \sum_{l=0}^n I^l \otimes H_h \otimes I^{n-l}$ and $H_{c,n} := \sum_{l=0}^n I^l \otimes H_c \otimes I^{n-l}$ respectively. Then, the initial thermal state is the i.i.d. Gibbs state $\left(\frac{e^{-\beta_h H_h}}{\text{tr } e^{-\beta_h H_h}}\right)^{\otimes n} \otimes \left(\frac{e^{-\beta_c H_c}}{\text{tr } e^{-\beta_c H_c}}\right)^{\otimes n} = \frac{e^{-\beta_h H_h^{\otimes n} - \beta_c H_c^{\otimes n}}}{(\text{tr } e^{-\beta_h H_h - \beta_c H_c})^n}$ with the inverse temperatures

$\beta_h, \beta_c > 0$. It is easy to check that Assumption 2.1 is satisfied since $\phi_n(\beta_h, \beta_c) = \log(\text{tr } e^{-\beta_h H_h - \beta_c H_c})^n = n \log \text{tr } e^{-\beta_h H_h - \beta_c H_c} = n\phi(\beta_h, \beta_c)$. Indeed, because $\phi(\beta_h, \beta_c) = \log \text{tr } e^{-\beta_h H_h - \beta_c H_c}$ is smooth, Assumption 2.1 is satisfied. In this case, the deviation from the extensivity is exactly 0. Hence, the achievability in Sec. 4 is verified. In fact, although the paper [19] gives a slightly different operation as the asymptotically optimal operation by using the specific structure of i.i.d. and gives a better estimation of the bound, the application of our general theory also gives the same estimation up to the second order as follows. Then, FGCB becomes

$$\Delta W \leq \left(1 - \frac{\beta_h}{\beta_c}\right) \Delta Q_{h,n} - C_{AA} \frac{\Delta Q_{h,n}^2}{n} + o\left(\frac{\Delta Q_{h,n}^2}{n}\right), \quad (9.1)$$

where ΔW and $\Delta Q_{h,n}$ are the extracted work and the endothermic heat from the hot bath respectively. Since there is no correlation between two baths, the matrix composed of the canonical correlations is just a diagonal matrix

$$(g_{ij}(\beta_c, \beta_h))_{ij} = \begin{pmatrix} \sigma_L^2 & 0 \\ 0 & \sigma_H^2 \end{pmatrix}, \quad (9.2)$$

where $\sigma_{L,H}^2$ is the variance of the energy of each bath at each initial inverse temperature. Thus, its inverse is

$$(g^{ij}(\beta_c, \beta_h))_{ij} = \begin{pmatrix} \sigma_L^{-2} & 0 \\ 0 & \sigma_H^{-2} \end{pmatrix}. \quad (9.3)$$

Therefore, the coefficient C_{AA} is calculated as

$$C_{AA} = \frac{1}{2} \left(\frac{g^{11}(\beta_c, \beta_h) \beta_h^2}{(\beta_c)^3} + \frac{g^{22}(\beta_c, \beta_h)}{\beta_c} \right) = \frac{\beta_h^2}{2\sigma_L^2 \beta_c^3} + \frac{1}{2\sigma_H^2 \beta_c}, \quad (9.4)$$

which indeed reproduces the second order coefficient [19, Eq. (39)].

9.2 1D Ising model

Next, we investigate an engine with heat baths composed of 1-dimensional (1D) Ising spin chain. Both the hot and the cold baths consist of n particles of 1D Ising spin chain, whose respective Hamiltonians $H_n^{(h)}$ and $H_n^{(c)}$ are given as

$$H_n^{(b)} = -J_b \left(\sum_{i=1}^{n-1} \hat{s}_i^{(b)} \hat{s}_{i+1}^{(b)} + \hat{s}_n^{(b)} \hat{s}_1^{(b)} \right), \quad (b = h, c) \quad (9.5)$$

where $\hat{s}_i^{(b)}$ is the spin z -component operator at site i of the hot ($b = h$) or the cold ($b = c$) bath, and J_b is its coupling constant. The initial state of the baths is the Gibbs state

$$\tau_{(\beta_h, \beta_c)}^{(n)} = \frac{e^{-\beta_h H_n^{(h)} - \beta_c H_n^{(c)}}}{\text{tr } e^{-\beta_h H_n^{(h)} - \beta_c H_n^{(c)}}}, \quad (9.6)$$

where β_h and β_c are the inverse temperatures of the hot and the cold baths respectively. The scaling is given by the number n of the spins, which is an example of non-i.i.d. scaling. The partition function $\mathcal{Z}_n^{(b)}(\beta_b)$ of the 1D Ising model is easily calculated by the transfer matrix

$$T = \begin{pmatrix} e^{\beta_b J_b} & e^{-\beta_b J_b} \\ e^{-\beta_b J_b} & e^{\beta_b J_b} \end{pmatrix} \quad (9.7)$$

as follows [48]:

$$\begin{aligned}
& \mathcal{Z}_n^{(b)}(\beta_b) \\
&= \sum_{s_1, \dots, s_n = -1, 1} e^{\beta_b J_b (\sum_{i=1}^{n-1} s_i s_{i+1} + s_n s_1)} \\
&= \text{tr } T^n = (2 \sinh \beta_b J_b)^n + (2 \cosh \beta_b J_b)^n \\
&= (2 \cosh \beta_b J_b)^n [1 + \tanh^n \beta_b J_b] \\
&= (2 \cosh \beta_b J_b)^n [1 + o(1)].
\end{aligned} \tag{9.8}$$

Thus, the free entropy of the baths is obtained as

$$\begin{aligned}
& \phi_n(\beta_h, \beta_c) \\
&= \log \mathcal{Z}_n^{(h)}(\beta_h) \mathcal{Z}_n^{(c)}(\beta_c) \\
&= n(\log[2 \cosh \beta_h J_h] + \log[2 \cosh \beta_c J_c]) + o(1),
\end{aligned} \tag{9.9}$$

and the asymptotic extensivity is verified.

Then, for the work extraction ΔW and the heat $\Delta Q_{h,n}$ from the hot bath, the following FGCB holds:

$$\Delta W \leq \left(1 - \frac{\beta_h}{\beta_c}\right) \Delta Q_{h,n} - C \frac{\Delta Q_{h,n}^2}{n} + o\left(\frac{\Delta Q_{h,n}^2}{n}\right). \tag{9.10}$$

To obtain the coefficient C , it is enough to calculate the asymptotic density σ_h^2 and σ_c^2 of the variance of the energy of the baths since the asymptotic density $g^{ij}(\beta_h, \beta_c)$ of the inverse matrix of the Fisher information is similar as that of the i.i.d. case (9.3). These are obtained as

$$\sigma_b^2 = \frac{J_b^2}{\cosh^2 \beta_b J_b} \quad (b = h, c). \tag{9.11}$$

Thus, we have

$$\begin{aligned}
C &= \frac{1}{2} \left(\frac{g^{11}(\beta_h, \beta_c) \beta_h^2}{(\beta_c)^3} + \frac{g^{22}(\beta_h, \beta_c)}{\beta_c} \right) \\
&= \frac{\beta_h^2}{2\sigma_c^2 \beta_c^3} + \frac{1}{2\sigma_h^2 \beta_c} \\
&= \frac{\beta_h^2 \cosh^2 \beta_c J_c}{2\beta_c^3 J_c^2} + \frac{\cosh^2 \beta_h J_h}{2\beta_c J_h^2}.
\end{aligned} \tag{9.12}$$

This formula implies that the absolute value of the coupling constant J_b directly affects the optimal performance in the finite-size regime. Especially, for fixed temperatures, the coefficient C takes its minimum when J_b satisfies

$$2\beta_b J_b \sinh 2\beta_b J_b - \cosh 2\beta_b J_b - 1 = 0, \tag{9.13}$$

which gives the best choice of J_b for the work extraction. On the other hand, since the sign of J_b makes no difference, the optimal performance does not depend on whether the system is ferromagnetic or anti-ferromagnetic.

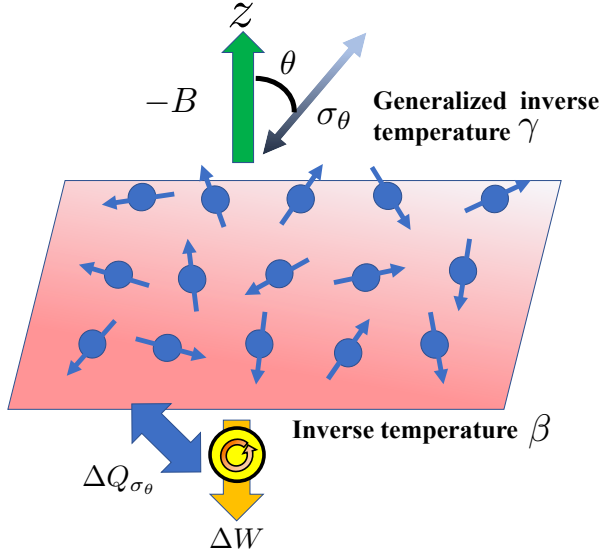


Figure 9.1: Schematic of spin- $\frac{1}{2}$ bath

9.3 Spin- $\frac{1}{2}$ bath

The next example is a simple toy model to illustrate the explicit behavior of the coefficient of the finite-size effect in FGCB with non-commutative quantities in a two-level system. We consider the work extraction from just one bath composed of spin- $\frac{1}{2}$ systems without interaction (Fig. 9.1) in the following model. n particles with spin- $\frac{1}{2}$ are placed on a lattice, so that each particle does not move. We assume that interactions among particles are negligible. We impose a uniform external magnetic field in z -direction, then the Hamiltonian of each particle is $H = \hbar\omega\sigma_z$, where $\sigma_z = |0\rangle\langle 0| - |1\rangle\langle 1|$, and 2ω is the cyclotron frequency. In this example, Quantity A is the energy given by this Hamiltonian. As seen from FGCB, by using another conserved quantity B , we can extract work even from one bath. As a toy model, we consider the spin in another direction as Quantity B . Obviously, since this system is symmetric with respect to the rotation around z -axis, it is sufficient to consider the angle $0 \leq \theta \leq \frac{\pi}{2}$ between the spin and z -axis. Then, we denote the θ -direction spin by

$$\sigma_\theta = \cos\theta(|0\rangle\langle 0| - |1\rangle\langle 1|) + \sin\theta(|0\rangle\langle 1| + |1\rangle\langle 0|). \quad (9.14)$$

We suppose that the bath is thermalized to the generalized thermal state

$$\tau_{\beta,\gamma}^{(n)} = \left(\frac{e^{-\beta H - \gamma \sigma_\theta}}{\mathcal{Z}} \right)^{\otimes n} \quad (9.15)$$

like the grand canonical ensemble with the non-commutative charges σ_θ and H [15], where $\beta > 0$ is the ordinary inverse temperature of the bath, and γ is the corresponding generalized inverse temperature for σ_θ . Here, γ is taken to be dimensionless. Although it is unclear whether such a thermal state can be realized physically in this way, this is one of the simplest examples of a generalized heat engine with two distinct conserved quantities. Since it is simple to calculate the coefficient of the second order term in FGCB for this example, we can analytically observe the behavior of the finite-size effects on its optimal performance. The free entropy is calculated as

$$\phi_n(\beta, \gamma) = n \log \mathcal{Z} = n(\log \cosh \sqrt{(\beta\hbar\omega)^2 + \gamma^2 + 2\gamma\beta\hbar\omega \cos\theta} + \log 2). \quad (9.16)$$

We use this state as the initial state of the bath. Note that in the commutative case $\theta = 0$, $\sigma_0 = \sigma_z$ is proportional to H , which means that σ_0 and H are essentially the same quantities. Hence, σ_0 is useless for the work extraction. Thus, in this system, non-commutativity is needed for the work extraction.

For the work extraction ΔW under the supply $\Delta Q_{\sigma_\theta, n} = o(n)$ of the θ -direction spin, the FGCB takes the following form:

$$\Delta W_n \leq -\frac{\gamma}{\beta} \Delta Q_{\sigma_\theta, n} - C(\beta, \gamma, \omega, \theta) \frac{(\Delta Q_{\sigma_\theta, n})^2}{n} + O\left(\frac{(\Delta Q_{\sigma_\theta, n})^3}{n^2}\right). \quad (9.17)$$

The coefficient $C_\theta(\beta, \gamma; \omega)$ is calculated by (3.13) as

$$C(\beta, \gamma, \omega, \theta) = \frac{((\beta \hbar \omega)^2 + \gamma^2 + 2\gamma\beta \hbar \omega \cos \theta)^{\frac{3}{2}}}{2\beta^3 (\hbar \omega)^2 \sin^2 \theta \tanh \sqrt{(\beta \hbar \omega)^2 + \gamma^2 + 2\gamma\beta \hbar \omega \cos \theta}}. \quad (9.18)$$

Note that this coefficient explicitly depends on the full parameters: the direction θ and cyclotron frequency 2ω as well as inverse temperatures. As already mentioned in the general theory, the coefficient $C(\beta, \gamma, \omega, \theta)$ reflects the correlation between the Hamiltonian and θ direction spin. Thus, while just the ratio $\frac{\gamma}{\beta}$ between the inverse temperatures determines the maximum work extraction in thermodynamic limit, the imposed field and the direction θ of the spin themselves explicitly make differences in consideration of finite-size regime.

To extract the work as large as possible, we should minimize $C(\beta, \gamma, \omega, \theta)$ under the fixed $\eta := \frac{\gamma}{\beta}$ to keep the first term. Then, the coefficient $C(\beta, \gamma, \omega, \theta)$ is rewritten as

$$C(\beta, \omega, \theta; \eta) := C(\beta, \beta\eta, \omega, \theta) = \frac{((\hbar \omega)^2 + \eta^2 + 2\hbar \omega \eta \cos \theta)^{\frac{3}{2}}}{2(\hbar \omega)^2 \sin^2 \theta \tanh\left(\beta \sqrt{(\hbar \omega)^2 + \eta^2 + 2\hbar \omega \eta \cos \theta}\right)}. \quad (9.19)$$

Interestingly, it depends on not only the ratio η , but also the single inverse temperature β . When η (hence the first term) is fixed, the lower the temperature is, the smaller $C(\beta, \omega, \theta; \eta)$ becomes. Moreover, $C(\beta, \omega, \theta; \eta)$ quite differently behaves in accordance with the sign of η (i.e. of γ) as follows.

At first, we consider the case when $\eta > 0$. In this case, $\Delta Q_{\sigma_\theta, n} < 0$ is needed to extract work. The coefficient $C(\beta, \omega, \theta; \eta)$ diverges $+\infty$ as $\theta \rightarrow 0$. The coefficient $C(\beta, \omega, \theta; \eta)$ always takes its minimum at $\theta = \frac{\pi}{2}$ (x -direction) for any β and ω :

$$C(\beta, \omega, \frac{\pi}{2}; \eta) = \frac{(\hbar^2 \omega^2 + \eta^2)^{\frac{3}{2}}}{2\hbar^2 \omega^2 \tanh\left(\beta \sqrt{\hbar^2 \omega^2 + \eta^2}\right)}. \quad (9.20)$$

The derivative of (9.20) with respect to ω is

$$\frac{\partial}{\partial \omega} C(\beta, \omega, \frac{\pi}{2}; \eta) = \frac{\hbar^4 \omega^4 - \hbar^2 \omega^2 \eta^2 - 2\eta^4}{\hbar^3 \omega^3 \sqrt{\hbar^2 \omega^2 + \eta^2} \tanh\left(\beta \sqrt{\hbar^2 \omega^2 + \eta^2}\right)} - \frac{\beta(\hbar^2 \omega^2 + \eta^2)}{\hbar \omega \sinh^2(\beta \sqrt{\hbar^2 \omega^2 + \eta^2})}. \quad (9.21)$$

Thus, further the value (9.20) takes its minimum at the ω_m such that the RHS of (9.21) vanishes. At large enough β , i.e. low enough temperature $T := k_B^{-1} \beta^{-1}$, where k_B is the Boltzmann constant, we have $\hbar \omega_m \approx \sqrt{2}\eta$ since the second term in (9.21) becomes negligible. Thus, in summary, to make the maximum work large, one should use x -direction spin and low temperature T , and tune ω to $\omega_m \approx \sqrt{2}\eta$. As an example, we show the graph of $C(\beta, \omega, \frac{\pi}{2}; \eta)$ as a function of θ at $T = 1\text{K}$, and $\eta = 1\text{J}$ in Fig. 9.2, which

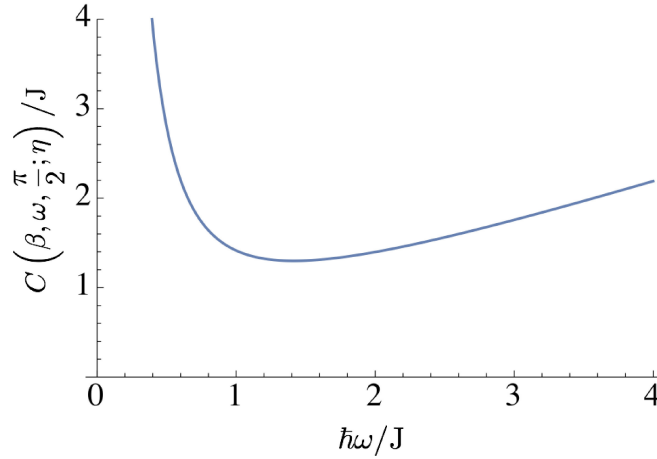


Figure 9.2: The graph of $C(\beta, \omega, \frac{\pi}{2}; \eta)$ at $T = 1\text{K}$, and $\eta = 1\text{J}$ as a function of ω . It takes its minimum at $\hbar\omega \approx \sqrt{2}J = \sqrt{2}\eta$.

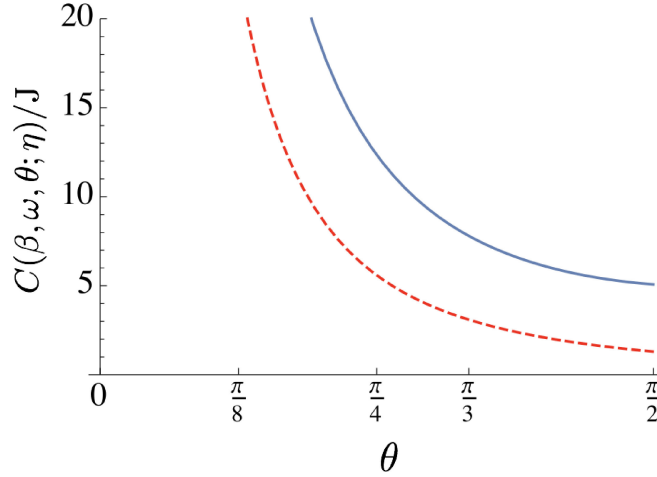


Figure 9.3: The graph of $C(\beta, \omega, \theta; \eta)$ at $T = 1\text{K}$, and $\eta = 1\text{J}$ with $\hbar\omega = 10\text{J}$ (solid blue curve) and $\hbar\omega = \sqrt{2}J$ (dashed red curve).

indeed takes its minimum at $\hbar\omega \approx \sqrt{2}J = \sqrt{2}\eta$. We also plot the graph of $C(\beta, \omega, \theta; \eta)$ as a function of θ at the same T and η with $\hbar\omega = 10\text{J}$ (solid blue curve) and $\hbar\omega = \sqrt{2}J$ (dashed red curve) in Fig. 9.3, which shows that $C(\beta, \omega, \theta; \eta)$ indeed becomes smaller when $\hbar\omega = \sqrt{2}\eta$.

Next, we consider the case when $\eta < 0$, where $\Delta Q_{\sigma_\theta, n}$ have to be positive to extract work. In this case, $\lim_{\theta \rightarrow 0} C(\beta, \omega, \theta; \eta) = (2\beta)^{-1}$ only when $\hbar\omega = -\eta$, otherwise it diverges to $+\infty$. Thus, a kind of resonance occurs. Since $C(\beta, \omega, \theta; \eta) > (2\beta)^{-1}$ holds in general, that gives the infimum of the drawback. Note that, however, $(2\beta)^{-1}$ is not the *minimum* since σ_θ with $\theta = 0$ can no longer be used for the work extraction. That is because H is proportional to $\sigma_0 = \sigma_z$. Thus, in summary, to make the maximum work large, one should tune ω to $-\eta$, and to use low temperature, small but non-zero θ . As an example, we show the graph of $C(\beta, \omega, \theta; \eta)$ as a function of θ at $T = 1\text{K}$, and $\eta = -1\text{J}$ with resonant $\hbar\omega = 1\text{J} = -\eta$ (dashed red curve) and non-resonant $\hbar\omega = \sqrt{2}J$ (solid blue curve) in Fig. 9.4. It shows that the coefficient indeed becomes small in $\theta \rightarrow 0$ for the resonant ω .

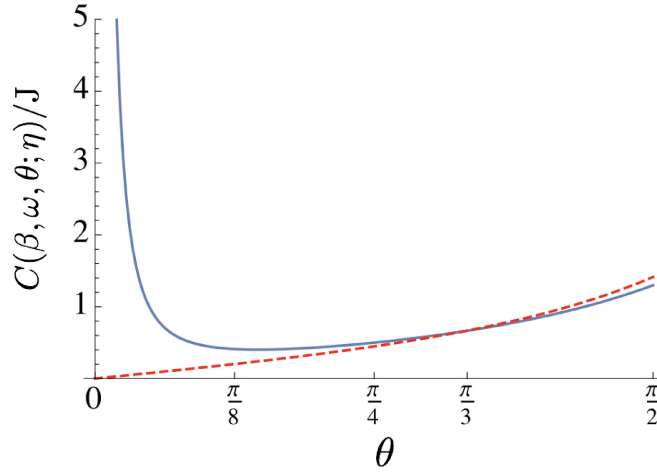


Figure 9.4: The graph of $C(\beta, \omega, \theta; \eta)$ as a function of θ at $T = 1\text{K}$, and $\eta = -1\text{J}$. As $\theta \rightarrow 0$, it becomes small for the resonant frequency $\hbar\omega = 1\text{J} = -\eta$ (dashed red curve), while it diverges for a non-resonant frequency $\hbar\omega = \sqrt{2}\text{J}$ (solid blue curve).

9.4 Heat engine with two baths exchanging particles

The next simple example is the heat engine exchanging not only energy but also particles between two baths, which may be used to model some electric cell, particle transportation, etc. This is a first example of continuous scaling not based on i.i.d. particles.

9.4.1 General observation of the model

Let the bath system $\mathcal{H}_{\text{Baths}}$ be split into the cold bath $\mathcal{H}_{\text{Bath},c}$ and the hot bath $\mathcal{H}_{\text{Bath},h}$. Each $\mathcal{H}_{\text{Bath},b}$ ($b = c, h$) has the Hamiltonian $H_{b,\lambda}$ and the number operator $N_{b,\lambda}$ with a scale parameter λ as follows:

$$H_{b,\lambda} = \sum_{\mathbf{n}=(n_1, n_2, \dots, n_{L_\lambda})} \left(\sum_{i=1}^{L_{b,\lambda}} E_{b,\lambda}(i) n_i \right) |\mathbf{n}\rangle\langle\mathbf{n}| \quad (9.22)$$

$$N_{b,\lambda} = \sum_{\mathbf{n}=(n_1, n_2, \dots, n_{L_\lambda})} \left(\sum_{i=1}^{L_{b,\lambda}} n_i \right) |\mathbf{n}\rangle\langle\mathbf{n}|, \quad (9.23)$$

where $E_{b,\lambda}(i)$ is the i -th energy level, $L_{b,\lambda}$ is the number of levels of the Hamiltonian. The initial state is the grand canonical Gibbs state with the initial generalized inverse temperature $\boldsymbol{\theta}_0 = (\beta_c, \beta_h, -\beta_c\mu_c, -\beta_h\mu_h)$ with $\beta_c > \beta_h$:

$$\tau_{\boldsymbol{\theta}_0}^{(\lambda)} = \frac{e^{-\beta_c H_{c,\lambda} + \beta_c \mu_c N_{c,\lambda}}}{\text{tr} e^{-\beta_c H_{c,\lambda} + \beta_c \mu_c N_{c,\lambda}}} \otimes \frac{e^{-\beta_h H_{h,\lambda} + \beta_h \mu_h N_{h,\lambda}}}{\text{tr} e^{-\beta_h H_{h,\lambda} + \beta_h \mu_h N_{h,\lambda}}}, \quad (9.24)$$

where $\beta_b > 0$ and μ_b are the inverse temperature and the chemical potential of $\mathcal{H}_{\text{Bath},b}$ ($b = c, h$), respectively. Thus, each bath works as a heat and particle bath simultaneously. Once the Assumption 2.1 is verified, we have the following FGCB for the work (energy) extraction ΔW under the endothermic heat $\Delta Q_{h,\lambda} = o(\lambda)$ from the hot bath and the particle number $\Delta N_{b,\lambda} = o(\lambda)$ absorbed from the bath

$\mathcal{H}_{\text{Bath},b}$ ($b = c, h$):

$$\begin{aligned}
& \Delta W \\
& \leq \left(1 - \frac{\beta_h}{\beta_c}\right) \Delta Q_{h,\lambda} + \mu_c \Delta N_{c,\lambda} + \frac{\beta_h}{\beta_c} \mu_h \Delta N_{h,\lambda} \\
& \quad - C_{HH} \frac{\Delta Q_{h,\lambda}^2}{\lambda} - \sum_{b=c,h} C_{NN}^{b,b} \frac{\Delta N_{b,\lambda}^2}{\lambda} - C_{NN}^{c,h} \frac{\Delta N_{c,\lambda} \Delta N_{h,\lambda}}{\lambda} - \sum_{b=c,h} C_{HN}^b \frac{\Delta Q_{h,\lambda} \Delta N_{b,\lambda}}{\lambda} \\
& \quad + o\left(\frac{\beta_h^2 \Delta Q_{h,\lambda}^2 + \Delta N_{c,\lambda}^2 + \Delta N_{h,\lambda}^2}{\lambda}\right), \tag{9.25}
\end{aligned}$$

where the signs of $\Delta Q_{h,\lambda}$ and $\Delta N_{b,\lambda}$ ($b = c, h$) are taken positive if they are absorbed from the bath to the engine. The coefficients are given as

$$C_{HH} = \frac{1}{2\beta_c} \left[\frac{\sigma_{N_h}^2}{\sigma_{H_h}^2 \sigma_{N_h}^2 - V_{HN}^{(h)2}} + \frac{\beta_h^2}{\beta_c^2} \frac{\sigma_{N_c}^2}{\sigma_{H_c}^2 \sigma_{N_c}^2 - V_{HN}^{(c)2}} \right] \tag{9.26}$$

$$C_{NN}^{h,h} = \frac{1}{2\beta_c} \left[\frac{\sigma_{H_h}^2}{\sigma_{N_h}^2 \sigma_{H_h}^2 - V_{HN}^{(h)2}} + \frac{\beta_h^2 \mu_h^2}{\beta_c^2} \frac{\sigma_{N_c}^2}{\sigma_{H_c}^2 \sigma_{N_c}^2 - V_{HN}^{(c)2}} \right] \tag{9.27}$$

$$C_{NN}^{c,c} = \frac{1}{2\beta_c} \left[\frac{\sigma_{H_c}^2}{\sigma_{N_c}^2 \sigma_{H_c}^2 - V_{HN}^{(c)2}} + \mu_c^2 \frac{\sigma_{N_c}^2}{\sigma_{H_c}^2 \sigma_{N_c}^2 - V_{HN}^{(c)2}} - 2\mu_c \frac{V_{HN}^{(c)}}{\sigma_{H_c}^2 \sigma_{N_c}^2 - V_{HN}^{(c)2}} \right] \tag{9.28}$$

$$C_{HN}^h = -\frac{1}{\beta_c} \left[\frac{\beta_h^2 \mu_h}{\beta_c^2} \frac{\sigma_{N_c}^2}{\sigma_{H_c}^2 \sigma_{N_c}^2 - V_{HN}^{(c)2}} + \frac{V_{HN}^{(h)}}{\sigma_{H_h}^2 \sigma_{N_h}^2 - V_{HN}^{(h)2}} \right] \tag{9.29}$$

$$C_{HN}^c = \frac{1}{\beta_c} \left[\frac{\beta_h}{\beta_c} \frac{V_{HN}^{(c)}}{\sigma_{H_c}^2 \sigma_{N_c}^2 - V_{HN}^{(c)2}} - \frac{\beta_h \mu_c}{\beta_c} \frac{\sigma_{N_c}^2}{\sigma_{H_c}^2 \sigma_{N_c}^2 - V_{HN}^{(c)2}} \right] \tag{9.30}$$

$$C_{NN}^{c,h} = \frac{1}{\beta_c} \left[\frac{\beta_h \mu_h \mu_c}{\beta_c} \frac{\sigma_{N_c}^2}{\sigma_{H_c}^2 \sigma_{N_c}^2 - V_{HN}^{(c)2}} - \frac{\beta_h \mu_h}{\beta_c} \frac{V_{HN}^{(c)}}{\sigma_{H_c}^2 \sigma_{N_c}^2 - V_{HN}^{(c)2}} \right], \tag{9.31}$$

where $\sigma_{H_b}^2$, $\sigma_{N_b}^2$ and $V_{HN}^{(b)}$ are the respective asymptotic densities of the variance $\text{Var}[A] := \text{tr} A^2 \tau_{\theta_0}^{(\lambda)} - (\text{tr} A \tau_{\theta_0}^{(\lambda)})^2$ and covariance $\text{Cov}[A, B] := \text{tr} AB \tau_{\theta_0}^{(\lambda)} - (\text{tr} A \tau_{\theta_0}^{(\lambda)})(\text{tr} B \tau_{\theta_0}^{(\lambda)})$ of each quantity defined as $\sigma_{H_b(N_b)}^2 := \lim_{\lambda \rightarrow \infty} \text{Var}[H_{b,\lambda}(N_b)]/\lambda$, $V_{HN}^{(b)} := \lim_{\lambda \rightarrow \infty} \text{Cov}[H_{b,\lambda}, N_{b,\lambda}]/\lambda$ ($b = c, h$). Thus, we obtain the explicit form of dependence of the optimal performance on the fluctuation of the energy and the particle number as well as their correlation in the coefficients of the finite-size effect.

On the other hand, we have the following FGCB for the particle number extraction ΔN_{tot} under the endothermic heat $\Delta Q_{b,\lambda}$ from $\mathcal{H}_{\text{Bath},b}$ ($b = c, h$) and the particle number $\Delta N_{h,\lambda}$ absorbed from one bath,

say hot bath:

$$\begin{aligned}
& \Delta N_{\text{tot}} \\
& \leq \left(1 - \frac{\beta_h \mu_h}{\beta_c \mu_c}\right) \Delta N_{h,\lambda} + \mu_c^{-1} \Delta Q_{c,\lambda} + \frac{\beta_h}{\beta_c \mu_c} \Delta Q_{h,\lambda} \\
& \quad - \tilde{C}_{HH} \frac{\Delta N_{h,\lambda}^2}{\lambda} - \sum_{b=c,h} \tilde{C}_{NN}^{b,b} \frac{\Delta Q_{b,\lambda}^2}{\lambda} - \tilde{C}_{NN}^{c,h} \frac{\Delta Q_{c,\lambda} \Delta Q_{h,\lambda}}{\lambda} - \sum_{b=c,h} \tilde{C}_{HN}^b \frac{\Delta N_{h,\lambda} \Delta Q_{b,\lambda}}{\lambda} \\
& \quad + o\left(\frac{\Delta N_{h,\lambda}^2 + \beta_c^2 \Delta Q_{c,\lambda}^2 + \beta_h^2 \Delta Q_{h,\lambda}^2}{\lambda}\right), \tag{9.32}
\end{aligned}$$

where the coefficients are similarly calculated.

9.4.2 A concrete model: an ideal Fermi gas inside the one dimensional well potential

As a concrete model, we consider an ideal Fermi gas. Let each bath $\mathcal{H}_{\text{Bath},b}$ ($b = c, h$) be composed of an ideal Fermi gas inside the infinite well potential

$$V_{b,\lambda}(x) = \begin{cases} 0 & (x \in [0, \lambda l_b]) \\ \infty & (x \notin [0, \lambda l_b]) \end{cases}, \tag{9.33}$$

where l_b is the length parameter to determine the rate of the size between two baths. λ is a dimensionless scaling parameter. For simplicity, we set l_b as the unit length for both baths. In this case, the energy eigenvalues of one particle is given by

$$E_{b,\lambda}(i) := E_\lambda(i) = \frac{\hbar^2 \pi^2 i^2}{2m\lambda^2} =: \frac{E_0}{\lambda^2} i^2 \quad (i = 1, 2, \dots), \tag{9.34}$$

where m is the mass of the particle. Moreover, we introduce a cut-off energy E to this Hamiltonian such that $E_\lambda(i) \leq E$. That is because the dimension should be finite to apply our general theory, strictly speaking. Nevertheless, with large enough E , this toy model can be an approximation of the true square well potential. In this case, the number L_λ of levels becomes finite, which is written as

$$L_\lambda = \max_{\frac{E_0}{\lambda^2} i^2 \leq E} i = \left\lfloor \sqrt{\frac{E}{E_0}} \lambda \right\rfloor. \tag{9.35}$$

Then, the free entropy of the bath $\mathcal{H}_{\text{Bath},b}$ ($b = c, h$) satisfies the asymptotic form

$$\begin{aligned}
& \phi_{b,\lambda}(\beta_b, \mu_b) \\
& = \log \sum_{(n_1, n_2, \dots, n_{L_\lambda}) \in \{0,1\}^{L_{0,\lambda}}} \prod_{i=1}^{L_\lambda} e^{\beta_b(-E_\lambda(i) + \mu_b)n_i} \\
& = \frac{\lambda}{2\sqrt{E_0}} \int_0^E \epsilon^{-\frac{1}{2}} \log(1 + e^{\beta_b \mu_b - \beta_b \epsilon}) d\epsilon + \mathcal{O}(1) \\
& = \int_0^E \frac{\lambda \sqrt{2m}}{2\pi \hbar} \epsilon^{-\frac{1}{2}} \log(1 + e^{\beta_b \mu_b - \beta_b \epsilon}) d\epsilon + \mathcal{O}(1) \\
& =: \lambda \phi_b(\beta_b, \mu_b) + \mathcal{O}(1). \tag{9.36}
\end{aligned}$$

Thus, Assumption 2.1 is satisfied with smaller deviation from the extensivity than $\mathcal{O}(\lambda^{\frac{1}{2}})$. Moreover, since the relations $\|H_{b,\lambda}\| \leq EL_\lambda = \mathcal{O}(\lambda)$ and $\|N_{b,\lambda}\| = L_\lambda = \mathcal{O}(\lambda)$ also hold, all the conditions for the achievability for Theorem 4.1 are verified. Hence this is indeed an example where the maximum work extraction in FGCB (9.25) is achievable.

Now, we further calculate the second order coefficients (9.26)-(9.31) in FGCB (9.25) in low temperature approximation. Supposing that E is sufficiently large, we regard E as ∞ . The asymptotic density of the energy ϵ_b and the particle number n_b are given as

$$\epsilon_b = \frac{\sqrt{2m}}{2\pi\hbar} \int_0^\infty \frac{\epsilon^{\frac{1}{2}}}{e^{\beta_b \epsilon - \beta_b \mu_b} + 1} d\epsilon \quad (9.37)$$

$$n_b = \frac{\sqrt{2m}}{2\pi\hbar} \int_0^\infty \frac{\epsilon^{-\frac{1}{2}}}{e^{\beta_b \epsilon - \beta_b \mu_b}} d\epsilon. \quad (9.38)$$

For sufficiently low temperature where $1 \ll \mu_b \beta_b$ holds, $I := \int_0^\infty \frac{F(\epsilon)}{e^{\beta_b \epsilon - \beta_b \mu_b}} d\epsilon$ is approximated as

$$I \approx \int_0^{\mu_b} F(\epsilon) d\epsilon + \frac{\pi^2}{6} \beta_b^{-2} F'(\mu_b). \quad (9.39)$$

Then, ϵ_b and n_b are approximated as

$$\epsilon_b = \frac{\sqrt{2m}}{2\pi\hbar} \mu_b^{-\frac{1}{2}} \left[\frac{2}{3} \mu_b^2 + \frac{\pi^2}{12} \beta_b^{-2} \right] \quad (9.40)$$

$$n_b = \frac{\sqrt{2m}}{2\pi\hbar} \mu_b^{\frac{1}{2}} \left[2 - \frac{\pi^2}{12} \beta_b^{-2} \mu_b^{-2} \right]. \quad (9.41)$$

Calculating their derivatives, we obtain the variances and correlation as

$$\sigma_{H_b}^2 = \frac{\sqrt{2m}}{2\pi\hbar} \frac{8\beta_b^2 \mu_b^2 + \pi^2}{8\beta_b^3 \mu_b^{\frac{1}{2}}} \quad (9.42)$$

$$\sigma_{N_b}^2 = \frac{\sqrt{2m}}{2\pi\hbar} \frac{8\beta_b^2 \mu_b^2 + \pi^2}{8\beta_b^3 \mu_b^{\frac{5}{2}}} \quad (9.43)$$

$$V_{HN}^{(b)} = \frac{\sqrt{2m}}{2\pi\hbar} \frac{24\beta_b^2 \mu_b^2 - \pi^2}{24\beta_b^3 \mu_b^{\frac{3}{2}}}. \quad (9.44)$$

We should consider the finite-size effect under the fixed first order coefficients, namely we fix $r := \beta_h/\beta_c$,

μ_h and μ_c . Then, we obtain the second order coefficients as follows:

$$C_{HH} = \frac{9\hbar\beta_c^2}{\sqrt{2m\pi}} \left[r^2 \mu_c^{\frac{1}{2}} \frac{8\beta_c^2 \mu_c^2 + \pi^2}{24\beta_c^2 \mu_c^2 + \pi^2} + r^3 \mu_h^{\frac{1}{2}} \frac{8\beta_c^2 r^2 \mu_h^2 + \pi^2}{24\beta_c^2 r^2 \mu_h^2 + \pi^2} \right] \quad (9.45)$$

$$C_{NN}^{h,h} = \frac{9\hbar\beta_c^2}{\sqrt{2m\pi}} \left[r^2 \mu_h^2 \mu_c^{\frac{1}{2}} \frac{8\beta_c^2 \mu_c^2 + \pi^2}{24\beta_c^2 \mu_c^2 + \pi^2} + r^3 \mu_h^{\frac{5}{2}} \frac{8\beta_c^2 r^2 \mu_h^2 + \pi^2}{24\beta_c^2 r^2 \mu_h^2 + \pi^2} \right] \quad (9.46)$$

$$C_{NN}^{c,c} = \frac{24\pi\hbar\mu_c^{\frac{5}{2}}\beta_c^2}{\sqrt{2m}(24\beta_c^2\mu_c^2 + \pi^2)} \quad (9.47)$$

$$C_{NN}^{c,h} = \frac{24\pi\hbar r \mu_h \mu_c^{\frac{3}{2}} \beta_c^2}{\sqrt{2m}(24\beta_c^2\mu_c^2 + \pi^2)} \quad (9.48)$$

$$C_{HN}^h = -\frac{6\hbar\beta_c^2}{\sqrt{2m\pi}} \left[3r^2 \mu_h \mu_c^{\frac{1}{2}} \frac{8\beta_c^2 \mu_c^2 + \pi^2}{24\beta_c^2 \mu_c^2 + \pi^2} + r^3 \mu_h^{\frac{3}{2}} \frac{24\beta_c^2 r^2 \mu_h^2 - \pi^2}{24\beta_c^2 r^2 \mu_h^2 + \pi^2} \right] \quad (9.49)$$

$$C_{HN}^c = -\frac{24\pi\hbar r \mu_c^{\frac{3}{2}} \beta_c^2}{\sqrt{2m}(24\beta_c^2\mu_c^2 + \pi^2)}. \quad (9.50)$$

According to these coefficients, it is remarkable that the optimal performance with finite-size effects explicitly depends on the mass m of the particle. It implies that heavier particles have better performance for heat engines. According to the interpretation of the finite-size effect as mentioned shortly after Theorem 3.1, this feature implies that the large mass leads to small response of the baths due to the large inertia.

10 Conclusion

We have revealed the effects of the finiteness of the baths with arbitrary multiple conserved quantities on the optimal performance of the generalized heat engine. We have extended the scaling to the generic form, imposing the extensivity. Under this generic scaling, we have derived FGCB as a fine-grained upper bound on the performance of generalized heat engines. FGCB includes the second order terms of order $\mathcal{O}\left(\frac{\|\mathbf{Q}_\lambda\|^2}{\lambda}\right)$ as the finite-size effect. Contrary to the thermodynamic limit regime, the coefficients of this finite-size effects terms reflect the canonical correlations between the multiple conserved quantities of the baths as well as the generalized inverse temperatures. The finite-size effect reflects the degradation of the performance caused by the linear response of the inverse temperature to the variation in the conserved quantities. It has turned out that the smaller the response becomes, the better performance is achieved.

FGCB has been given for the implicit-battery formulation for wide applicability of the theory. However, to show the achievability of FGCB, we should construct a protocol under the explicit-battery formulation. We have imposed independence of the state of the battery on the explicit-battery operations as the no-cheating condition to guarantee that the battery really works only as a storage of extracted work, but not as an entropy sink. In this sense, the energy transfer to the battery is indeed work-like. Under the conservation laws, the cyclicity of the working body, and the no-cheating condition, we have explicitly constructed a protocol with an explicit battery. Our protocol has been given by a permutation of the basis of the baths, which works independently of the detail of the system. Though the equality in FGCB is attained by the thermal state at the ideal final inverse temperature θ_λ which is determined by the conditions (3.23)-(3.26), this state cannot necessarily be obtained from the initial thermal state through the operations in finite-size bath. Instead, the resultant state of our protocol is very close to

this ideal thermal state. The closeness in terms of the relative entropy shows that our protocol indeed achieves the equality in FGCB up to $o\left(\frac{\|\mathbf{Q}_\lambda\|^2}{\lambda}\right)$, which is negligible in our regime. We have shown this estimation by making use of the information geometric structure. One of the technical key points is the extension of the central limit theorem, which is needed for the strong large deviation estimation for our generic scaling, whose detail has been given in Sec. 5 and 7. In our protocol, the dynamics on the working body \mathcal{H}_C is trivial, and completely split from the baths and the battery. Thus, no catalytic effects work in this asymptotically optimal protocol, which means that the improvement of the optimal performance by catalytic effects is of order $o\left(\frac{\|\mathbf{Q}_\lambda\|^2}{\lambda}\right)$. However, note that the working body \mathcal{H}_C should be needed to physically realize the dynamics even if the resultant map per one cycle is trivial like our protocol.

Strictly speaking, we have imposed additional conditions in Theorem 4.1. One is on the order of the norm of each quantity as (4.3). Since this condition is needed just for a technical reason, it is possibly removed in future works. The others are the conditions (4.1) and (4.2) that the order of the deviation from the extensivity (2.5), (2.6) is sufficiently small as $\mathcal{O}(\lambda^\alpha)$ with $\alpha < \frac{1}{2}$. This is possibly more essential in a physical sense, since great deal of the deviation from the extensivity of each quantity possibly degrades the performance of the engine. Further investigation is needed to reveal such an effects caused by the deviation from the extensivity on the performance of protocols. In addition, to verify that our protocol achieves the optimal performance in our analysis, it is also needed that we run the engine with the heat of the order $\lambda^{\frac{5}{8}} \ll \|\mathbf{Q}_\lambda\| \ll \lambda$. This condition is required to verify that the relative entropy between the ideal final thermal state and the final state of our protocol is small enough. It is a future work to further investigate the relation between the amount of generalized heat and the scale. It is an interesting feature that the quality of the protocol may alter according to its amount of the generalized heat. Furthermore, it remains to verify the relation between the work fluctuation and the performance, though this is also important in order to investigate the realistic usefulness of the heat engine [49, 50].

Our protocols have similar forms for both commutative and non-commutative cases. Nevertheless, only the average conservation is satisfied for non-commutative case, though the strict conservation law is satisfied for the commutative case. While the validity of the average conservation law for the protocol may depend on the initial state in general, our protocol satisfies the conservation law regardless of the initial state of the battery and working body, just depending on the baths. Although our protocol for the non-commutative case indefinitely uses coherence, it may be revived if some resource of coherence is appropriately included in our operation as pointed out by [34]. Giving protocols for multiple non-commutative quantities under strictly conservation law is an important open but challenging problem.

Finally, we have applied our general results to some examples. 1D Ising spin chain was a first example for the non-i.i.d. scaling with asymptotic extensivity. We have shown that the coupling constant of the spin chain affects the optimal performance for the finite baths. Especially, the best value of the coupling constant gives the largest optimal performance. On the other hand, even the finite-size effect is independent of whether the spin chain is ferromagnetic or anti-ferromagnetic. In the example of a two-level system heat engine, we have analytically investigated the behavior of the coefficient of the finite-size effect. We have revealed interesting structures of its finite-size regime, which is quite different from the thermodynamic limit, such as a resonance. As a more physical example, we have considered a heat engine with an ideal gas exchanging particles. Though it is so famous canonical example, it was for the first time to explicitly calculate the coefficients of the finite-size-effect terms in the optimal performance of that heat engine. For an ideal Fermi gas inside a well potential, we have found that these coefficients explicitly depend on the mass of the particle, which is again quite different from the nature in thermodynamic limit. This fact implies that heavier particles have better performance for heat engines. From these examples, we have already seen that the finite-size effect depends on the peculiar parameters for each model such as the

coupling constant, external field, and mass in various ways. It is an important future work to investigate the finite-size effect for more practical heat engines in detail, and to compare it with our general result.

Our protocol may be hard to experimentally realize since it involves in microscopic control of the baths' basis. Thus, a realistic protocol should be considered as a future work. Recently, a realization of thermal operations (with infinite baths) by realistic operations was studied [51]. Though that result cannot be directly applied to the finite-size regime, our protocol may be realized by some combination of realistic operations. Then, our model may be applicable to an electric battery, or biological systems in a realistic mesoscopic scale.

Since our analysis is based on the asymptotic analysis of finite-size systems, the obtained results clarify the optimal performance of mesoscopic systems. We consider that our analysis is a first step to universal understanding of quantum thermodynamics in various scale.

A Information geometry for density matrices

In this section, we review the detail of the information geometric analysis in the proof of Lemma 4.1 in Sec. 4.4 including non-commutative case. At first, we give a brief review on the information geometry based on the theory of the Bregman divergence. This theory gives an abstract framework for the information geometry. Then, we can use the results from this theory just by applying it to individual cases. Next, we do so for our case.

A.1 The Bregman divergence

We review an abstract framework of information geometry in terms of the Bregman divergence [52]. The meaning of the following abstraction will become clear when we apply this theory to our state family in the next subsection.

We consider a twice-differentiable strictly convex function μ defined on an open subset Θ of \mathbb{R}^D . The set Θ usually corresponds to the parameter space of the states in consideration. Then, we define the Bregman divergence of μ as

$$D^\mu(\bar{\theta}||\theta) := \sum_{k=1}^D \frac{\partial \mu}{\partial \theta^k}(\bar{\theta})(\bar{\theta}^k - \theta^k) - \mu(\bar{\theta}) + \mu(\theta). \quad (\text{A.1})$$

The Bregman divergence is a 'distance measure' of the abstract parameter space Θ induced by μ , which is called a potential function. It is an advantage of the abstract theory that once we find such a potential function μ , we can apply all the results based on μ .

Since μ is strictly convex, $\theta \mapsto \eta(\theta) := \nabla \mu(\theta)$ is one-to-one. Thus, η gives another parametrization. Because μ plays the role of the free entropy, its derivatives $\eta_k = \frac{\partial \mu}{\partial \theta^k}$ correspond to the expectation values. The Bregman divergence can be expressed by this dual parameter. To do so, we observe the Legendre transformation ν of μ

$$\nu(\eta) := \max_{\tilde{\theta}} \left[\sum_k \eta_k \tilde{\theta}^k - \mu(\tilde{\theta}) \right]. \quad (\text{A.2})$$

Then, the Bregman divergence $D^\nu(\eta||\bar{\eta})$ for ν is also defined since ν is also a strictly convex function of η . When $\eta = \nabla \mu(\theta)$, we have

$$\nu(\eta) = \sum_k \eta_k \theta^k - \mu(\theta) \quad (\text{A.3})$$

by the definition. Using this relation for $\eta = \nabla\mu(\theta)$ and $\bar{\eta} = \nabla\mu(\bar{\theta})$, we obtain

$$\begin{aligned}
D^\mu(\bar{\theta}||\theta) &= \sum_k \bar{\eta}_k(\bar{\theta}^k - \theta^k) - \mu(\bar{\theta}) + \mu(\theta) = \sum_k \theta^k(\eta_k - \bar{\eta}_k) + \left(\sum_k \bar{\eta}_k \bar{\theta}^k - \mu(\bar{\theta}) \right) - \left(\sum_k \eta_k \theta^k - \mu(\theta) \right) \\
&= \sum_k \theta^k(\eta_k - \bar{\eta}_k) + \nu(\bar{\eta}) - \nu(\eta) = D^\nu(\eta||\bar{\eta}) \\
&= \int_0^1 \sum_{k,j} (\eta_k - \bar{\eta}_k)(\eta_j - \bar{\eta}_j) \frac{\partial^2 \nu}{\partial \eta_k \partial \eta_j} (\bar{\eta} + (\bar{\eta} - \eta)t) dt, \tag{A.4}
\end{aligned}$$

where the last line follows from the Taylor's formula. It should be remarked that the matrix $(\frac{\partial^2 \nu}{\partial \eta_k \partial \eta_j}(\eta))_{kj}$ is verified to be the inverse of $(\frac{\partial^2 \mu}{\partial \theta^k \partial \theta^j}(\theta))_{kj}$ from the chain rule and the inverse relation $\theta^k = \frac{\partial \nu}{\partial \eta_k}(\eta)$.

With a point $\theta' \in \Theta$ and l linearly independent vectors $v_1, \dots, v_l \in \mathbb{R}^D$, an l -dimensional flat $\mathcal{E} = \{\theta \in \Theta | \theta = \theta' + \sum_{j=1}^l a^j v_j, (a^1, a^2, \dots, a^l) \in \mathbb{R}^l\}$ is defined. Such a flat \mathcal{E} is called an exponential subfamily of Θ whose generator is $\{v_1, \dots, v_l\}$. As the name indicates, this is an abstraction of exponential family, i.e. a family of generalized thermal states. As a 'dual flat' of the exponential subfamily \mathcal{E} , $\mathcal{M} = \{\theta \in \Theta | b_j = \sum_{i=1}^D v_j^i \eta_i(\theta) \ (j = 1, \dots, l)\}$ with some fixed real numbers b_1, \dots, b_l is called a mixture subfamily of Θ whose generator is $\{v_1, \dots, v_l\}$. The definition of a mixture subfamily means that \mathcal{M} is a flat with respect to the dual parameter η . Hence, \mathcal{M} corresponds to the state family with fixed expectation values. Then, the following Pythagorean theorem [37] for the Bregman divergence holds:

Proposition A.1 (Amari [53]). *Let \mathcal{M} be an mixture subfamily of Θ whose generator is $\{v_1, \dots, v_l\}$. For an arbitrary point $\theta \in \Theta$, there exists a unique intersection θ^* between \mathcal{M} and the exponential subfamily \mathcal{E} containing θ with the same generator $\{v_1, \dots, v_l\}$. This θ^* satisfies the following:*

1. For any point $\theta' \in \mathcal{M}$, $D^\mu(\theta' || \theta) = D^\mu(\theta' || \theta^*) + D^\mu(\theta^* || \theta)$ holds.
2. $\theta^* = \arg \min_{\theta' \in \mathcal{M}} D^\mu(\theta' || \theta)$.

A.2 Application of the Pythagorean theorem to the state family

Now, we apply the above abstract theory of the Bregman divergence to our situation. First of all, we parametrize all of the full-rank states of $\mathcal{H}_{\text{Baths}}$ as follows. Since the set of all Hermitian matrices on $\mathcal{H}_{\text{Baths}}$ can be seen as a real vector space whose dimension is $D + 1 := d_\lambda(d_\lambda + 1)/2$, there exists a basis $\{E_1, E_2, \dots, E_{D+1}\}$, where we omit the label λ on D for simplicity of the notation. Because the observables $A_{i,\lambda}$, $B_{i,\lambda}$ ($i = 1, 2$) of the baths and the identity matrix I are linearly independent Hermitian matrices, we can take the basis $\{E_1, E_2, \dots, E_D\}$ such that $E_1 = A_{1,\lambda}$, $E_2 = A_{2,\lambda}$, $E_3 = B_{1,\lambda}$, $E_4 = B_{2,\lambda}$, and $E_{D+1} = I$. Then, the parametrization $\exp\left(\sum_{i=1}^{D+1} \xi^i E_i\right) / \text{tr} \exp\left(\sum_{i=1}^{D+1} \xi^i E_i\right)$ of the states by $(\xi^1, \xi^2, \dots, \xi^{D+1}) \in \mathbb{R}^{D+1}$ runs all the full-rank states ρ since $\log \rho$ is Hermitian, and $\sum_{i=1}^{D+1} \xi^i E_i$ runs all the Hermitian matrices. However, this parametrization is still redundant in the sense that for any $a \in \mathbb{R}$, (ξ_1, \dots, ξ_D, a) corresponds to the same state $\rho(\xi_1, \dots, \xi_D) := \exp\left(\sum_{i=1}^D \xi^i E_i\right) / \text{tr} \exp\left(\sum_{i=1}^D \xi^i E_i\right)$ since

$$\frac{\exp\left(\sum_{i=1}^D \xi^i E_i + aI\right)}{\text{tr} \exp\left(\sum_{i=1}^D \xi^i E_i + aI\right)} = \frac{e^a \exp\left(\sum_{i=1}^D \xi^i E_i\right)}{e^a \text{tr} \exp\left(\sum_{i=1}^D \xi^i E_i\right)} = \rho(\xi_1, \dots, \xi_D). \tag{A.5}$$

Hence, we employ the parametrization $\rho(\xi) = \exp\left(\sum_{i=1}^D \xi^i E_i\right) / \text{tr} \exp\left(\sum_{i=1}^D \xi^i E_i\right)$ by $\xi = (\xi_1, \dots, \xi_D) \in \mathbb{R}^D$, so that the parameter space is $\Theta = \mathbb{R}^D$. The potential function is $\mu(\xi) := \log \text{tr} \exp\left(\sum_{i=1}^D \xi^i E_i\right)$. Indeed, it is a twice-differentiable strictly convex function, which can be verified by observing that its Hessian matrix $(\frac{\partial^2 \mu}{\partial \xi^i \partial \xi^j}(\xi))_{ij}$ is positive definite as follows. The Hessian matrix is equal to the matrix $(K_{i,j}(\xi))_{ij}$ composed of the canonical correlations

$$K_{i,j}(\xi) := \int_0^1 ds \text{tr} \rho(\xi)^{1-s} (E_i - \eta_i(\xi)) \rho(\xi)^s (E_j - \eta_j(\xi)) \quad (\text{A.6})$$

between E_i and E_j , where $\eta_i(\xi) := \frac{\partial \mu}{\partial \xi^i}(\xi)$ is equal to the expectation value $\text{tr} \rho(\xi) E_i$ of E_i . Thus, it is sufficient to show the positivity of $(K_{i,j}(\xi))_{ij}$. To do so, we firstly observe that the canonical correlation is a positive definite inner product:

Lemma A.1. *Let ρ be a state with full-rank. Then, for any matrix X , we have $\int_0^1 ds \text{tr} \rho^{1-s} X \rho^s X \geq 0$. In addition, $\int_0^1 ds \text{tr} \rho^{1-s} X \rho^s X = 0$ if and only if $X = 0$.*

Proof. Using the commutativity inside of the trace, we obtain

$$\text{tr} \rho^{1-s} X \rho^s X = \text{tr} \rho^{\frac{1-s}{2}} \rho^{\frac{1-s}{2}} X \rho^{\frac{s}{2}} \rho^{\frac{s}{2}} X = \text{tr} \left(\rho^{\frac{1-s}{2}} X \rho^{\frac{s}{2}} \right) \left(\rho^{\frac{s}{2}} X \rho^{\frac{1-s}{2}} \right) = \text{tr} \left(\rho^{\frac{s}{2}} X \rho^{\frac{1-s}{2}} \right)^\dagger \left(\rho^{\frac{s}{2}} X \rho^{\frac{1-s}{2}} \right) \geq 0 \quad (\text{A.7})$$

for any $0 < s < 1$. If $\text{tr} \left(\rho^{\frac{s}{2}} X \rho^{\frac{1-s}{2}} \right)^\dagger \left(\rho^{\frac{s}{2}} X \rho^{\frac{1-s}{2}} \right) = 0$, then $\rho^{\frac{s}{2}} X \rho^{\frac{1-s}{2}} = 0$ holds. Since ρ is invertible, ρ^t ($0 < t < 1$) is also. Then, $X = \rho^{-\frac{s}{2}} \rho^{\frac{s}{2}} X \rho^{\frac{1-s}{2}} \rho^{-\frac{1-s}{2}} = 0$. \square

Then, we show the positivity:

Lemma A.2. *$(K_{i,j}(\xi))_{ij}$ is positive definite for any $\xi \in \mathbb{R}^D$.*

Proof. For any vector $(a^1, \dots, a^D) \in \mathbb{R}^D$, we have

$$\sum_{i,j=1}^D a^i K_{i,j}(\xi) a^j = \int_0^1 ds \text{tr} \rho(\xi)^{1-s} X \rho(\xi)^s X, \quad (\text{A.8})$$

where $X = \sum_{i=1}^D a^i (E_i - \eta_i(\xi))$. Hence, $\sum_{i,j=1}^D a^i K_{i,j}(\xi) a^j \geq 0$ follows from Lemma A.1. If $\sum_{i,j=1}^D a^i K_{i,j}(\xi) a^j = 0$, $\sum_{i=1}^D a^i (E_i - \eta_i(\xi)) = 0$ holds again by Lemma A.1. Then, since E_i ($i = 1, \dots, D$) and I are linearly independent, $(a^1, \dots, a^D) = 0$ follows from the expression

$$\sum_{i=1}^D a^i E_i - \left[\sum_{i=1}^D a^i \eta_i(\xi) \right] I = 0. \quad (\text{A.9})$$

Thus, $(K_{i,j}(\xi))_{ij}$ is a positive definite matrix. \square

Thus, $\mu(\xi)$ is verified to be strictly convex. The Bregman divergence associated with $\mu(\xi)$ is nothing but the relative entropy as follows:

$$\begin{aligned} D^\mu(\bar{\xi} \parallel \xi) &= \sum_{k=1}^D \frac{\partial \mu}{\partial \xi^k}(\bar{\xi}) (\bar{\xi}^k - \xi^k) - \mu(\bar{\xi}) + \mu(\xi) = \sum_{k=1}^D \text{tr} \rho(\bar{\xi}) E_k (\bar{\xi}^k - \xi^k) - \mu(\bar{\xi}) + \mu(\xi) \\ &= \text{tr} \rho(\bar{\xi}) (\log \rho(\bar{\xi}) - \log \rho(\xi)) = D(\rho(\bar{\xi}) \parallel \rho(\xi)). \end{aligned} \quad (\text{A.10})$$

The exponential subfamily $\mathcal{E} := \{\xi \in \mathbb{R}^D | \xi = \sum_{i=1}^4 \theta^i v_i, \boldsymbol{\theta} = (\theta^1, \theta^2, \theta^3, \theta^4) \in \mathbb{R}^4\}$ with its generator $v_1 = (1, 0, \dots, 0)$, $v_2 = (0, 1, 0, \dots, 0)$, $v_3 = (0, 0, 1, 0, \dots, 0)$, $v_4 = (0, 0, 0, 1, 0, \dots, 0)$ corresponds to the exponential family $\mathcal{E}_S := \{\tau_{\boldsymbol{\theta}}^{(\lambda)} | \boldsymbol{\theta} \in \mathbb{R}^4\}$ of the thermal states by observing

$$\tau_{\boldsymbol{\theta}}^{(\lambda)} = \frac{\exp\left[\sum_{i=1}^2 (\theta^i A_{i,\lambda} + \theta^{i+2} B_{i,\lambda})\right]}{\text{tr} \exp\left[\sum_{i=1}^2 (\theta^i A_{i,\lambda} + \theta^{i+2} B_{i,\lambda})\right]} = \frac{\exp\left[\sum_{i=1}^4 \theta^i E_i\right]}{\text{tr} \exp\left[\sum_{i=1}^4 \theta^i E_i\right]} = \frac{\exp\left[\sum_{k=1}^D \sum_{i=1}^4 \theta^i v_i^k E_k\right]}{\text{tr} \exp\left[\sum_{k=1}^D \sum_{i=1}^4 \theta^i v_i^k E_k\right]} = \rho\left(\sum_{i=1}^4 \theta^i v_i\right). \quad (\text{A.11})$$

On the other hand, the mixture subfamily $\mathcal{M} := \{\xi \in \mathbb{R}^D | b_j = \sum_{k=1}^D v_j^k \eta_k(\xi) \ (j = 1, 2, 3, 4)\}$ with the same generator v_1, v_2, v_3, v_4 corresponds to the state family $\mathcal{M}_S := \{\rho > 0 | \text{tr} \rho E_j = b_j, \ (j = 1, 2, 3, 4)\}$ whose expectation values of $A_{i,\lambda}$ and $B_{i,\lambda}$ are fixed because

$$b_j = \sum_{k=1}^D v_j^k \eta_k(\xi) = \sum_{k=1}^D v_j^k \text{tr} \rho(\xi) E_k = \text{tr} \rho(\xi) \sum_{k=1}^D v_j^k E_k = \text{tr} \rho(\xi) E_j \quad (j = 1, 2, 3, 4). \quad (\text{A.12})$$

Especially, for an arbitrary full-rank state ρ , the mixture subfamily \mathcal{M} with $b_j = \text{tr} \rho E_j$ corresponds to the state family whose expectation values of E_j are shared with ρ . We denote the corresponding state family of \mathcal{M} by $\mathcal{M}_S(\rho)$. Then, applying Proposition A.1 to \mathcal{M} and \mathcal{E} in terms of our Bregman divergence, relative entropy, we obtain the desired Pythagorean theorem for our situation:

Lemma A.3. *For an arbitrary full-rank state ρ , there exists a unique thermal state $\tau_{\boldsymbol{\theta}^*}^\lambda \in \mathcal{E}_S$ such that $\tau_{\boldsymbol{\theta}^*}^\lambda \in \mathcal{M}_S(\rho)$. Moreover, for an arbitrary thermal state $\tau_{\boldsymbol{\theta}}^\lambda \in \mathcal{E}_S$, we have*

$$D(\rho || \tau_{\boldsymbol{\theta}}^\lambda) = D(\rho || \tau_{\boldsymbol{\theta}^*}^\lambda) + D(\tau_{\boldsymbol{\theta}^*}^\lambda || \tau_{\boldsymbol{\theta}}^\lambda). \quad (\text{A.13})$$

Notice that Lemma A.3 is valid for both the non-commutative and commutative $A_{i,\lambda}$ and $B_{i,\lambda}$.

Furthermore, we can see the thermal states $\tau_{\boldsymbol{\theta}}^{(\lambda)}$ as a state family parametrized by the generalized inverse temperature $\boldsymbol{\theta}$. The relative entropy $D(\tau_{\boldsymbol{\theta}}^{(\lambda)} || \tau_{\boldsymbol{\theta}}^{(\lambda)})$ is again equal to the Bregman divergence associated with the free entropy $\phi_\lambda(\boldsymbol{\theta})$ as the strictly convex function on the parameter. Then, applying (A.4) to this Bregman divergence, we obtain

$$D(\tau_{\boldsymbol{\xi}}^{(\lambda)} || \tau_{\boldsymbol{\theta}}^{(\lambda)}) = \int_0^1 \sum_{ij} (\eta_{\lambda,i}(\boldsymbol{\theta}) - \eta_{\lambda,i}(\boldsymbol{\xi})) (\eta_{\lambda,j}(\boldsymbol{\theta}) - \eta_{\lambda,j}(\boldsymbol{\xi})) J_\lambda^{ij}(\mathbf{s}_\lambda(t)) t dt \quad (\text{A.14})$$

for any generalized inverse temperatures $\boldsymbol{\xi}$ and $\boldsymbol{\theta}$, where $\mathbf{s}_\lambda(t)$ is the generalized inverse temperature satisfying $\boldsymbol{\eta}_\lambda(\mathbf{s}_\lambda(t)) = t\boldsymbol{\eta}_\lambda(\boldsymbol{\theta}) + (1-t)\boldsymbol{\eta}_\lambda(\boldsymbol{\xi})$.

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