Measurement-based formulation of quantum heat engines

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There exist two formulations for quantum heat engines that model energy transfer between two microscopic systems. One is the semiclassical scenario and the other is the full quantum scenario. The former is formulated as unitary evolution for the internal system and is adopted by the statistical mechanics community. In the latter, the whole process is formulated as unitary and is adopted by the quantum information community. This paper proposes a model for quantum heat engines that transfer energy from a collection of microscopic systems to a macroscopic system like a fuel cell. In such a situation, the amount of extracted work is visible for a human. For this purpose, we formulate a quantum heat engine as the measurement process whose measurement outcome is the amount of extracted work. Under this model, we derive a suitable energy-conservation law and propose a more concrete submodel. Then we derive a trade-off relation between the measurability of the amount of work extraction and the coherence of the internal system, which limits the applicability of the semiclassical scenario to a heat engine transferring energy from a collection of microscopic systems to a macroscopic system.

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I. INTRODUCTION

Thermodynamics started as a study that clarifies the upper limit of the efficiency of macroscopic heat engines [1] and has become a huge realm of science that covers from electric batteries [2] to black holes [3]. Today, with the development of experimental techniques, the study of thermodynamics is reaching a new phase. The development of experimental techniques is realizing micromachines in the laboratory [4–6]. We cannot apply standard thermodynamics to these small-size heat engines as it is, because it is a phenomenological theory for macroscopic systems. In order to study such small-size heat engines, we need to use statistical mechanical approaches.

In the statistical mechanical approach, the internal system of the heat engine can be formulated as a system obeying time-dependent Hamiltonian dynamics, which is called the classical standard formulation in this paper. The classical standard formulation has been used since Einstein and Gibbs [7]. For example, Bochkov and Kuzolev [8–11] showed the second law under the standard formulation for cyclic operations and it was extended to general operations as a corollary of the Jarzynski equality [12]. In this way, the classical standard formulation works well for classical heat engines and has been adopted by the statistical mechanics community [13–18]. In the statistical mechanics community, as a quantum extension of the classical standard formulation, the work-extraction process was formulated to be unitary for the internal system, which is called the semiclassical scenario in this paper. As an example, employing this scenario, Lenard showed the second law for cyclic processes in the quantum setting [19]. Also, based on this scenario, Kurchan [20] and Tasaki [21] gave a quantum generalization of the Jarzynski equality. The semiclassical scenario has been adopted by the statistical mechanics community [22–34]. Here they assume that the time evolution of the internal system is unitary. On the other hand, researchers in the quantum information community recently discussed unitary dynamics of the whole system including the external system storing the extracted work [35–44], which is called the fully quantum scenario in this paper.[1] Although both models are different, Åberg (see Sec. II D in the Supplemental Material in [45]) showed that the internal unitary dynamics in the semiclassical scenario can be realized as the approximation of the unitary of the whole system.[2] So both models have succeeded in analyzing heat engines that transfer energy between two microsystems.

To further develop quantum thermodynamics, this paper discusses heat engines transferring discernible energy from a collection of quantum systems to a macroscopic system, which is a new frontier of quantum thermodynamics. This kind of heat engine is used in our daily life. As a typical example, fuel cells with microstructure have been developed recently as solid oxide fuel cells (SOFCs) [47–49]. A fuel cell has a collection of microscopic systems as an internal system and a macroscopic output power, which can be measured as the amount of extracted work by humans and affects our daily life, while the amount of extracted work does not need to be measured in the previous case, as shown in Fig. 1. As the next topic, in order to analyze such a fuel cell with microstructure as a quantum heat engine, it is interesting to develop a model for a heat engine that includes a measurement process to produce the output power. That is, it is an interesting study

[1]Our classification between the semiclassical scenario and the fully quantum scenario is based on the range of the unitary dynamics of our interest. Although the papers [35–43] discuss only states diagonal in energy basis, the unitary dynamics of their interest covers the whole system, including the external system storing the extracted work. Hence, we classify them as the fully quantum scenario.

[2]To realize the approximation of the unitary of the whole system, Åberg [45] employed the coherence in the external system storing the extracted work. Also, Åberg [45] showed that the coherence of the external system can be used repeatedly to perform coherent operations. As was commented in [46], when we repeatedly use the same external system, the overall coherent operation has diminished accuracy and is necessarily accompanied by an increased thermodynamic cost.

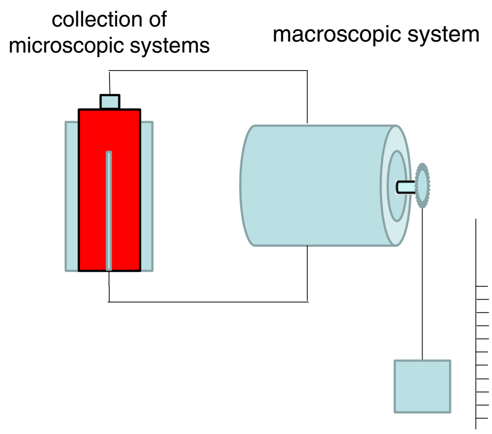

FIG. 1. Energy extraction from a collection of microscopic systems to a macroscopic system.

to treat the output power as a measurement outcome, i.e., to formulate the heat engine as a quantum measurement process for the quantum internal system. In this scenario, people do not measure the inside of the fuel cell, but measure alternatively the macroscopic object.

Indeed, the measurability of the amount of extracted work is a very crucial task due to the following real situation. Consider the case when an electric bill is charged by an electric power company. In fact, at the time of a disaster, a SOFC is intended to be used as an electric power source [50]. If the measured amount of extracted work is different from the true amount of extracted work, the user will not pay the electric bill because he or she cannot trust the amount charged. To avoid such trouble, we need to precisely measure the amount of extracted work as a fundamental requirement for our model of a heat engine. However, it is an open problem to extend quantum thermodynamics to such a case. That is, it is our desire to formulate our model for a quantum heat engine as the energy-extraction process that equips a quantum measurement process to output the amount of extracted work.

In the present article we propose a general formation of quantum heat engines based on quantum measurement theory [51,52] as completely positive (CP) work extraction, in which the total system is composed of the internal system and the external system, which can be regarded as a work storage system. As shown by Ozawa [52], such a quantum measurement process is realized by an indirect measurement process, that is, the combination of a unitary on the whole system and the measurement of the energy on the meter system, which is the work storage in the current situation. In this scenario, the initial unitary can be regarded as the fully quantum scenario [35–43]. So the initial unitary has to satisfy the energy-conservation law in the sense of the fully quantum scenario.

There are three issues to discuss about our model. First, it is not trivial to identify the energy-conservation law under our CP work-extraction model. To clarify a natural condition for energy conservation, we consider the natural energy-conservation law in the dynamics between the internal system and the quantum storage of the fully quantum model, which can be regarded as the first step of the measuring process in the indirect measurement model in the context of the CP work-extraction model [52]. When additionally we impose a natural constraint of the initial state for the quantum storage, we derive a very restrictive energy-conservation law in an unexpected way, which will be called the level-4 energy-conservation law (Theorem 1). That is, the restrictive condition is naturally obtained by considering the indirect measurement model and the existing energy-conservation law in the fully quantum model [37–43]. However, there is a case when this constraint is satisfied only partially. Under such conditions, we derive weaker conditions as other types of energy-conservation laws for CP work extractions.

Second, we need a more concrete model as a natural extension of the classical standard formulation [7] because the above CP work extraction is too abstract and contains an unnatural case when the dynamics of the internal system depends on the state of the external system, while the dynamics of the internal system is not independent of the state of the external system in the classical standard formulation [7]. Fortunately, Åberg (see Sec. II of the Supplemental Material in [45]) discussed a concrete model that satisfies this requirement as a fully quantum model with the energy-conservation law; we call the model the shift-invariant model because shift invariance guarantees the independence of the state of the external system. However, he did not discuss the measurability of the amount of extracted work because the main topic of his work was work coherence. So we investigate how to naturally convert the model to a CP work extraction with the level-4 energy-conservation law. Since the shift-invariant model is obtained from a semiclassical model in a canonical way, this model can be regarded as a modification of the semiclassical model. Under this modification, the semiclassical model works properly when we discuss the amount of extracted work and endothermic energy.

Third, we examine how the semiclassical scenario works approximately when the measurability of the amount of extracted work is imposed. Indeed, it has been expected that the fully quantum scenario converges to the semiclassical scenario in a proper approximation, although the semiclassical scenario assumes that the internal system evolves unitarily under a time-dependent Hamiltonian controlled by a classical external system. This examination checks this expectation. To discuss this issue, we investigate the trade-off between the approximation of the internal unitary and the measurability of the amount of extracted work. As a result, we derive two remarkable trade-off relations between information gain for knowing the amount of extracted work and the maintained coherence of the thermodynamic system during the work-extraction process. These trade-off relations clarify that we can hardly know the amount of extracted work when the time evolution of the internal system is close to unitary.

This paper is organized as follows. In Sec. II we formulate work extraction as a measurement process by using CP work extraction. We give four energy-conservation laws, level-1, level-2, level-3, and level-4 energy-conservation laws, among which the level-4 energy-conservation law is the most restrictive. In Sec. III we discuss fully quantum work extraction as a unitary process between the internal system and the work storage as well as the energy-conservation law. We discuss what kind of energy-conservation laws in the

CP work-extraction model are derived from the respective conditions for the fully quantum work extraction. In Sec. IV we introduce the shift-invariant model as a modification of the semiclassical model. We consider how well this model works as a model for a heat engine. In Sec. V we derive two remarkable trade-off relations between information gain for knowing the amount of extracted work and the maintained coherence of the thermodynamic system during the work extraction process. These trade-off relations clarify that we can hardly know the amount of extracted work when the time evolution of the internal system is close to unitary.

II. WORK EXTRACTION AS A MEASUREMENT PROCESS

In this section we give the basic idea of our measurement-based formulation of work extraction from a quantum system to a macroscopic system. Let us start with standard thermodynamics; in a macroscopic heat engine, the work is given as a discernible energy change of a macroscopic work storage. In our quantum setting, we extract energy from a collection of quantum systems to a macroscopic system. That is, a discernible energy change of a macroscopic work storage is caused by the effect of a collection of quantum systems. In quantum physics, such a macroscopic discernible influence caused by a quantum system can be described only by a measurement process as in Fig. 1. Therefore, we need to formulate work extraction from the quantum system to the macroscopic system as a measurement process.

Let us formulate the above idea more concretely. We consider a heat engine in which the internal system is a collection of microscopic systems and the meter system is a macroscopic system, which can be regarded as the output system of the heat engine. For example, a fuel battery has fuel cells as the internal system and the motor system as the meter system. Hence, as the internal system we consider a quantum system I, whose Hilbert space is $\mathcal{H}_I$. We refer to the Hamiltonian of I as $\hat{H}_I$. The internal system I usually consists of the thermodynamical system S and the heat baths $\{B_m\}_{m=1}^M$, but we do not discuss such detailed structure of the internal system I here. Let us formulate the work extraction from I. We assume that the amount of the work is indicated by a meter (Fig. 2).

In other words, we assume that we have equipment to assess the amount of extracted work and that the equipment indicates the work w_j with the probability p_j. In quantum mechanics, such a process that determines an indicated value a_j with the probability p_j is generally described as a measurement process. Thus, we formulate work extraction from the quantum system as a measurement process [52]. As the minimal

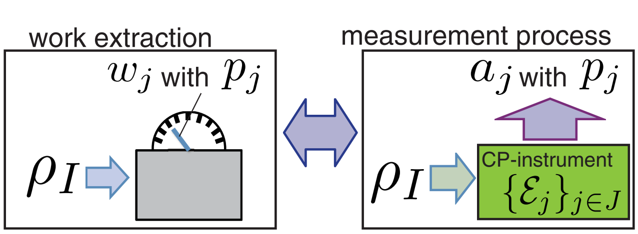

FIG. 2. Work extraction as a measurement process.

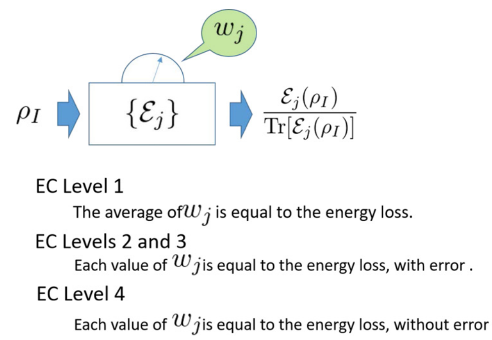

FIG. 3. Concepts of the energy-conservation laws.

requirement, we demand that the average of w_j is equal to the average energy loss of I during the measurement.

Definition 1 (CP work extraction). Let us take an arbitrary set of a CP instrument $\{\mathcal{E}_j\}_{j\in\mathcal{J}}$ and measured values $\{w_j\}_{j\in\mathcal{J}}$ satisfying the following conditions: (a) each $\mathcal{E}_j$ is a CP map, (b) $\sum_j \mathcal{E}_j$ is a completely positive and trace-preserving (CPTP) map, and (c) $\mathcal{J}$ is a discrete set of outcomes. When the set $\{\mathcal{E}_j,w_j\}_{j\in\mathcal{J}}$ satisfies the above condition, we refer to the set $\{\mathcal{E}_j,w_j\}_{j\in\mathcal{J}}$ as a CP work extraction.

Here we note that the measurement process $\{\mathcal{E}_j\}$ is not necessarily a measurement of the Hamiltonian of the internal system. It is not difficult to treat the case where $\mathcal{J}$ is a continuous set, but to avoid mathematical difficulty, we consider only the case where $\mathcal{J}$ is discrete. Since the heat engine needs to satisfy the conservation law of energy, we consider four kinds of energy-conservation laws for a CP work extraction $\{\mathcal{E}_j,w_j\}_{j\in\mathcal{J}}$ (Figs. 3 and 4). First, we consider the weakest condition.

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

$$\mathrm{Tr}\hat{H}_I\rho_I = \sum_j w_j \mathrm{Tr}\mathcal{E}_j(\rho_I) + \sum_j \mathrm{Tr}\hat{H}_I\mathcal{E}_j(\rho_I), \tag{1}$$

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

Since the level-1 energy-conservation law is too weak, as explained later, we introduce stronger conditions with an orthonormal basis $\{|x\rangle\}_x$ of $\mathcal{H}_I$ such that $|x\rangle$ is an eigenstate of the Hamiltonian $\hat{H}_I$ associated with the eigenvalue h_x. For

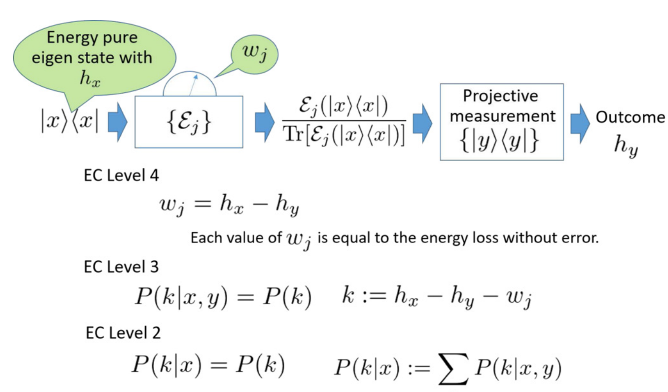

FIG. 4. Level-2, -3, and -4 energy-conservation laws.

this purpose, we introduce the spectral decomposition of $\hat{H}_I$ as $\hat{H}_I = \sum_h h P_h$, where P_h is the projection to the energy eigenspace of $\hat{H}_I$ whose eigenvalue is h.

Definition 3 (level-4 energy-conservation law). A CP work extraction $\{\mathcal{E}_j, w_j\}_{j\in\mathcal{J}}$ is called a level-4 CP work extraction when

$$\mathcal{E}_j(\Pi_x) = P_{h_x - w_j}\mathcal{E}_j(\Pi_x)P_{h_x - w_j} \tag{2}$$

for any initial eigenstate $\Pi_x := |x\rangle\langle x|$. This condition is called the level-4 energy-conservation law.

The meaning of (2) is that the resultant state $\frac{1}{\mathrm{Tr}\mathcal{E}_j(\Pi_x)}\mathcal{E}_j(\Pi_x)$ must be an energy eigenstate with energy $h_x - w_j$ because the remaining energy in the internal system is $h_x - w_j$. That is, the level-4 energy-conservation law requires the conservation of energy for every possible outcome j. One might consider that the level-4 energy-conservation law is too strong a constraint. However, as shown in Theorem 1, this condition holds if and only if the natural energy-conservation law holds as the dynamics between the internal system and the quantum storage of the full quantum model, which can be regarded as the first step of the measuring process in the indirect measurement model (Definition 6) and the initial state for the quantum storage is an energy eigenstate. Further, as precisely mentioned in Lemma 12, when the level-4 energy-conservation law holds, the measurement outcome precisely reflects the amount of energy lost from the internal system. So such a CP work extraction can be used for the purpose mentioned in the second paragraph of the Introduction.

However, there is a possibility that the initial state of the quantum storage is not an energy eigenstate. To characterize such a case, we introduce intermediate conditions in between the level-1 and level-4 energy-conservation laws. In Lemmas 4 and 8 we will clarify what physical situations in the indirect model correspond to these two conservation laws.

Here, to introduce two other energy-conservation laws, we introduce several notions for a CP work extraction $\{\mathcal{E}_j, w_j\}_{j\in\mathcal{J}}$. Let the initial state on I be an eigenstate $|x\rangle$. After the CP work extraction $\{\mathcal{E}_j, w_j\}_{j\in\mathcal{J}}$, we perform a measurement of $\{\Pi_y := |y\rangle\langle y|\}$ on the resultant system $\mathcal{H}_I$. We obtain the joint distribution $P_{JY|X}(j,y|x)$ of the two outcomes j and y as

$$P_{JY|X}(j,y|x) = \langle y|\mathcal{E}_j(\Pi_x)|y\rangle. \tag{3}$$

Then we introduce the random variable $K := h_X - h_Y - w_J$ that describes the difference between the loss of energy and the extracted energy. So we define the two distributions

$$P_{K|X}(k|x) := \sum_{j,y:h_x-h_y-w_j=k} P_{JY|X}(j,y|x), \tag{4}$$

$$P_{K|YX}(k|y,x) := \sum_{j:h_x-h_y-w_j=k} P_{J|YX}(j|y,x), \tag{5}$$

where

$$P_{J|YX}(j|y,x) := \frac{P_{JY|X}(j,y|x)}{\sum_j P_{JY|X}(j',y|x)}. \tag{6}$$

Definition 4 (level-2 and -3 energy-conservation laws). Now we introduce two energy-conservation laws for a CP work extraction $\{\mathcal{E}_j, w_j\}_{j\in\mathcal{J}}$ when the level-1 energy-conservation law holds. When the relation $P_{K|X}(k|x) = P_{K|X}(k|x')$ holds for k and $x \neq x'$, the CP work extraction $\{\mathcal{E}_j, w_j\}_{j\in J}$ is called a level-2 CP work extraction. Similarly, when the relation $P_{K|Y,X}(k|y,x) = P_{K|Y,X}(k|y',x')$ holds for k and $(x,y) \neq (x',y')$, the CP work extraction $\{\mathcal{E}_j, w_j\}_{j\in J}$ is called a level-3 CP work extraction. These conditions are called the level-2 and -3 energy-conservation laws.

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

$$P_{K|X}(k|x) = \delta_{k,0} \tag{7}$$

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

$$\mathcal{P}_{\hat{H}_I}(\rho) := \sum_h P_h \rho P_h. \tag{8}$$

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

$$\mathcal{P}_{\hat{H}_I}(\mathcal{E}_j(\rho)) = \mathcal{P}_{\hat{H}_I}(\mathcal{E}_j(\mathcal{P}_{\hat{H}_I}(\rho))) = \mathcal{E}_j(\mathcal{P}_{\hat{H}_I}(\rho)). \tag{9}$$

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

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

Proof. We employ the Kraus representation $\{A_{j,l}\}$ of $\mathcal{E}_j$,

$$\mathcal{E}_j(\rho) = \sum_l A_{j,l}\rho A_{j,l}^\dagger. \tag{10}$$

Then, due to the condition (2), $A_{j,l}$ has the form

$$A_{j,l} = \sum_h A_{j,l,h}, \tag{11}$$

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

$$P_h\mathcal{E}_j(\rho)P_h = \mathcal{E}_j\big(P_{h+w_j}\rho P_{h+w_j}\big) = P_h\mathcal{E}_j\big(P_{h+w_j}\rho P_{h+w_j}\big)P_h. \tag{12}$$

Taking the sum in h, we obtain (9). ∎

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

We also consider the following condition for a CP work extraction.

Definition 5 (CP unital work extraction). Consider a CP work extraction $\{\mathcal{E}_j, w_j\}_{j\in\mathcal{J}}$. When the CPTP map $\sum_j \mathcal{E}_j$ is unital, namely, when

$$\sum_j \mathcal{E}_j(\hat{1}_I) = \hat{1}_I \tag{13}$$

holds, we refer to the CP work extraction $\{\mathcal{E}_j, w_j\}_{j\in\mathcal{J}}$ as the CP unital work extraction.

Because an arbitrary unital map does not decrease the von Neumann entropy [53], the CP unital work extraction corresponds to the class of work extractions that do not decrease the entropy of I. That is, an arbitrary ρ_I satisfies

$$\Delta S_I := S\left(\sum_j \mathcal{E}_j(\rho_I)\right) - S(\rho_I) \geqslant 0, \tag{14}$$

where $S(\rho) := \mathrm{Tr}[-\rho \log \rho]$, and the base of the logarithmic function is e throughout this paper. In contrast, we have the following characterization of the entropy of the output random variable.

Lemma 2. Let $\{\mathcal{E}_j, w_j\}_{j\in\mathcal{J}}$ be a level-4 work extraction. We denote the random variable describing the amount of extracted work by W. Then, for any initial state ρ_I of the internal system, the resultant entropy $S[W]$ of the system W is

$$S[W] \leqslant 2 \log N, \tag{15}$$

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

One might consider that Lemma 2 is too weak to justify the unital condition. However, as shown in Theorem 2, the unital condition is a natural condition for CP work extraction.

Proof. Due to the condition for a level-4 work extraction, for a possible w_j there exist eigenstates x and x' such that $w_j = h_x - h_{x'}$. Hence, the number of possible w_j is less than N^2. Thus, we obtain (15). ■

When a CP work extraction is level 4 as well as unital, we refer to it as a standard CP work extraction for convenience of description because Theorems 1 and 2 guarantee that these conditions are satisfied under a natural setting as illustrated in a Venn diagram (Fig. 5) of the CP work extractions.

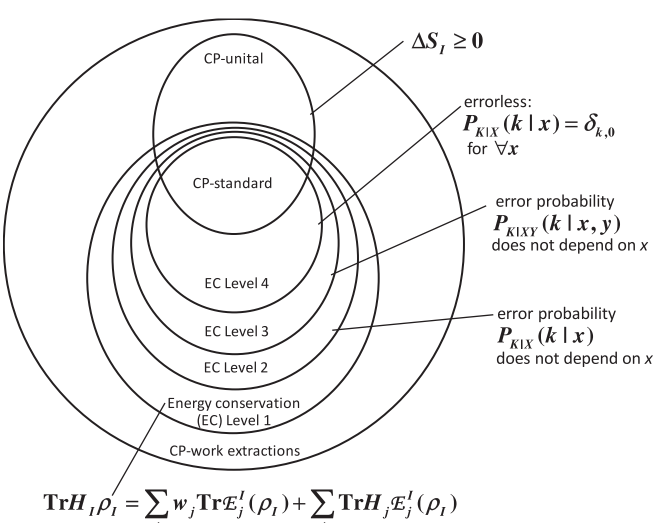

FIG. 5. Venn diagram of the CP work extractions.

III. FULLY QUANTUM WORK EXTRACTION

Next we consider the unitary dynamics of a heat engine between the internal system I and the external system E that stores the extracted work from I. This dynamics is essential for our CP work-extraction model as follows. Here the internal system I is assumed to interact only with E and the external system E is described by the Hilbert space $\mathcal{H}_E$ and has the Hamiltonian $\hat{H}_E$. In relation to the CP work-extraction model, this type of description of a heat engine is given as an indirect measurement process that consists of the following two steps [52]. The first step is the unitary time evolution U_{IE} that conserves the energy of the combined system IE and the second step is the measurement of the Hamiltonian $\hat{H}_E$. That is, the second step is given as the measurement corresponding to the spectral decomposition of the Hamiltonian $\hat{H}_E$. While previous works [35–43] have discussed the unitary time evolution U_{IE} with a proper energy-conservation law, the relation with the CP work-extraction model was not discussed.

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

$$\mathcal{E}_j(\rho_I) := \mathrm{Tr}_E U(\rho_I \otimes \rho_E) U^\dagger (\hat{1}_I \otimes P_{E,j}), \tag{16}$$

$$w_j := h_{E,j} - \mathrm{Tr}\hat{H}_E \rho_E. \tag{17}$$

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

Here any FQ work extraction corresponds to a CP work extraction. Conversely, considering the indirect model for an instrument model, we can show that there exists a FQ work extraction $\mathcal{F}$ with a pure state ρ_E for an arbitrary CP work extraction $\{\mathcal{E}_j, w_j\}_{j\in\mathcal{J}}$ such that $\mathrm{CP}(\mathcal{F}) = \{\mathcal{E}_j, w_j\}_{j\in\mathcal{J}}$ [52] (see also Theorem 5.7 in [54]).

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

Definition 7 (FQ energy-conservation law). When a unitary U is called energy conserving for the Hamiltonian $\hat{H}_I$ and $\hat{H}_E$,

$$[U, \hat{H}_I + \hat{H}_E] = 0. \tag{18}$$

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

The condition (18) is called the FQ energy-conservation law. Note that the above condition does not depend on the choice of the initial state ρ_E on the external system. Indeed, the condition (18) is equivalent to the condition

$$\begin{aligned}\mathrm{Tr}(\hat{H}_I + \hat{H}_E) U(\rho_I \otimes \rho_E) U^\dagger \\ = \mathrm{Tr}(\hat{H}_I + \hat{H}_E)(\rho_I \otimes \rho_E) \forall \rho_I, \rho_E.\end{aligned} \tag{19}$$

When we make restrictions on the state ρ_E, the condition (19) is weaker than the condition (18). For example, when the condition (19) is given with a fixed ρ_E, the CP work extraction CP($\mathcal{F}$) satisfies the level-1 energy-conservation law. However, such a restriction is unnatural, because such restricted energy conservation cannot recover the conventional energy conservation. Thus, we consider the condition (19) without any constraint on the state ρ_E. Hence, we have no difference between the condition (18) and the average energy-conservation law (19) in this scenario. Indeed, if we do not consider the measurement process on the external system E, the model given in Definition 7 corresponds to the formulations that are used in Refs. [37–43].

Here we discuss how to realize the unitary U satisfying (18). For this purpose, we prepare the following lemma.

Lemma 3. For an arbitrary small $\epsilon > 0$ and a unitary U satisfying (18), there exist a Hermitian matrix B and a time $t_0 > 0$ such that

$$\|B\| \leqslant \epsilon, \quad U = \exp[it_0(\hat{H}_I + \hat{H}_E + B)]. \tag{20}$$

Proof. Choose a Hermitian matrix C such that $\|C\| \leqslant \pi$ and $U = \exp(iC)$. Since C and $\hat{H}_I + \hat{H}_E$ commute, we can choose a common basis $\{|x\rangle\}$ of $\mathcal{H}_I \otimes \mathcal{H}_E$ that diagonalizes C and $\hat{H}_I + \hat{H}_E$ simultaneously. For any t, we can choose a set of integers $\{n_x\}$ such that $\|D_t\| \leqslant \pi$, where $D := C - t(\hat{H}_I + \hat{H}_E) - \sum_x 2\pi n_x |x\rangle\langle x|$. Hence, the Hermitian matrix $B := \frac{1}{t}D$ satisfies both conditions in (20) with $\epsilon = \frac{\pi}{t}$. So, choosing t large enough, we obtain the desired result. ∎

Due to Lemma 3, any unitary U satisfying (18) can be realized with a sufficiently long time t by adding the small interaction Hamiltonian term B. Note that the interaction B does not change in $0 < t < t_0$. Thus, in order to realize the unitary U, we only have to turn on the interaction B at $t = 0$ and to turn it off at $t = t_0$. From $t = 0$ to $t = t_0$, we do not have to control the total system IE time dependently. Namely, we can realize a "clockwork heat engine," which is programmed to perform the unitary transformation U automatically.

Now we have the following lemma.

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

Proof. For any j, due to the FQ energy-conservation law (18), we can choose j' such that

$$\langle x|U^\dagger(\hat{1}_I \otimes P_{E,j})|y\rangle = \langle x|(\hat{1}_I \otimes P_{E,j'})U^\dagger|y\rangle. \tag{21}$$

Then the FQ energy-conservation law (18) implies that

$$\begin{aligned} h_x - h_y - w_j &= h_x - h_y - h_{E,j} + \mathrm{Tr}\hat{H}_E\rho_E \\ &= -h_{E,j'} + \mathrm{Tr}\hat{H}_E\rho_E. \end{aligned} \tag{22}$$

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

$$\begin{aligned} P_{K|X}(k|x) &= \sum_{j,y:h_x-h_y-w_j=k} \mathrm{Tr}U(\Pi_x \otimes \rho_E)U^\dagger(\Pi_y \otimes P_{E,j}) \\ &= \sum_{\substack{j',y: \\ h_{E,j'} = -k + \mathrm{Tr}\hat{H}_E\rho_E}} \mathrm{Tr}U(\Pi_x \otimes \rho_E)(\hat{1}_I \otimes P_{E,j'})U^\dagger(\Pi_y \otimes \hat{1}_E) \\ &\overset{(a)}{=} \sum_{j':h_{E,j'}=-k+\mathrm{Tr}\hat{H}_E\rho_E} \mathrm{Tr}U(\Pi_x \otimes \rho_E)(\hat{1}_I \otimes P_{E,j'})U^\dagger(\hat{1}_I \otimes \hat{1}_E) \\ &= \sum_{j':h_{E,j'}=-k+\mathrm{Tr}\hat{H}_E\rho_E} \mathrm{Tr}(\Pi_x \otimes \rho_E)(\hat{1}_I \otimes P_{E,j'}) \\ &= \sum_{j':h_{E,j'}=-k+\mathrm{Tr}\hat{H}_E\rho_E} \mathrm{Tr}_E\rho_E P_{E,j'}, \end{aligned} \tag{23}$$

which does not depend on x, where (a) follows from the combination of (21) and (22). ∎

The external system interacts with the macroscopic outer system before and after the work extraction. So it is difficult to set the initial state ρ_E of the external system to a superposition of eigenstates of the Hamiltonian $\hat{H}_E$. Hence, it is natural to restrict the initial state ρ_E to be an eigenstate of the Hamiltonian $\hat{H}_E$. More generally, we restrict the initial state so that the support of the initial state ρ_E belongs to an eigenspace of the Hamiltonian $\hat{H}_E$.

Now we have the following theorem.

Theorem 1. Let $\mathcal{F} = (\mathcal{H}_E, \hat{H}_E, U, \rho_E)$ be an energy-conserving FQ work extraction. Then the support of the initial state ρ_E belongs to an eigenspace of the Hamiltonian $\hat{H}_E$ if and only if the CP work extraction CP($\mathcal{F}$) satisfies the level-4 energy-conservation law.

Proof. The support of the initial state ρ_E belongs to an eigenspace of the Hamiltonian $\hat{H}_E$. Due to the assumption, the probability $\mathrm{Tr}_E\rho_E P_{E,j'}$ takes a nonzero value only in the case when $h_{E,j'} = \mathrm{Tr}\hat{H}_E\rho_E$. Due to (23), the above condition is equivalent to the condition that the probability $P_{K|X}(k|x)$ has nonzero value only when $k = 0$. Hence, we obtain the desired equivalence relation. ∎

Finally, we have the following characterization of the entropy of the external system E.

Lemma 5. Let $\mathcal{F} = (\mathcal{H}_E, \hat{H}_E, U, \rho_E)$ be an energy-conserving FQ work extraction. We assume that ρ_E is a pure eigenstate of $\hat{H}_E$ and that the external system $\mathcal{H}_E$ has a nondegenerate Hamiltonian $\hat{H}_E$, i.e., $\hat{H}_E = \sum_j h_j \Pi_j$, where

$\Pi_j := |j\rangle\langle j|$. Then the entropy of the final state in the external system is

$$S(\mathrm{Tr}_I U(\rho_I \otimes \rho_E)U^\dagger) \leqslant \log 2N, \tag{24}$$

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

Proof. Due to Lemma 1, this FQ work extraction generates a CP work extraction satisfying the level-4 condition. So Lemma 2 guarantees (15). Since $\hat{H}_E$ is nondegenerate, the random variable W given in Lemma 2 satisfies

$$\begin{aligned} S[W] &= S\left(\sum_j \Pi_j \mathrm{Tr}_I U(\rho_I \otimes \rho_E)U^\dagger \Pi_j\right) \\ &\geqslant S(\mathrm{Tr}_I U(\rho_I \otimes \rho_E)U^\dagger). \end{aligned} \tag{25}$$

The combination of (15) of Lemma 2 and (25) yields (24). ■

IV. SHIFT-INVARIANT MODEL

The above CP work extraction and fully quantum work extraction are too abstract in comparison with the classical standard formulation. Also, these models contain the case when the dynamics of the internal system depends on the state of the external system, which seems unnatural. To discuss this issue, we recall the classical standard formulation [7–11,13–18]. In this scenario, we consider an external agent who performs the external operation as the classical time evolution f of the internal system I (which usually consists of the system S and the heat bath B). In this scenario, the loss of energy of the internal system can be regarded as the amount of extracted work due to the energy-conservation law. That is, when the initial state of the internal system x and the Hamiltonian is given as a function h, the amount of extracted work is $h(x) - h(f(x))$.

Note that the dynamics of the internal system does not depend on the state of the external system in the classical standard formulation. To discuss its quantum extension, we introduce a classification of Hamiltonians. A Hamiltonian $\hat{H}_I$ is called a lattice when there is a real positive number d such that any difference $h_i - h_j$ is an integer multiple of d, where $\{h_i\}$ is the set of eigenvalues of $\hat{H}_I$. When $\hat{H}_I$ is a lattice, the maximum d is called the lattice span of $\hat{H}_I$. Otherwise, it is called a nonlattice. In this section we assume that our Hamiltonian $\hat{H}_I$ is a lattice and denote the lattice span by h_E. In the lattice case, using the external system $E1$ with a doubly infinite Hamiltonian, Åberg (see Sec. II of the Supplemental Material in [45]) proposed a model in which the behavior of the heat engine depends less on the initial state of the external system. The external system $E1$ looks unphysical, because it does not have a ground state. When the dimension of the internal system is finite, he also reconstructed the property of $E1$ in a pair of harmonic oscillators (see Sec. IV-D in the Supplemental Material in [45]). So we employ this definition for the simplicity of mathematical use.

Although he discussed the catalytic property and the role of coherence based on this model, he did not discuss the relation with the CP work-extraction model. In particular, he did not deal with the trade-off relation between the coherence and the measurability of the amount of extracted work in this model because he discussed the average extracted work, but not the amount of the extracted work as measurement outcome. In this section we construct essentially the same model as Åberg [45] in a slightly different logical step in the lattice case and call it a shift-invariant model, while he did not give a clear name. Then we investigate the relation with the CP work-extraction model. In the next section we extend the model to the nonlattice case, while he did not discuss the nonlattice case. Later we discuss a trade-off relation.

Consider a nondegenerate external system $E1$. Let $\mathcal{H}_{E1}$ be $L^2(\mathbb{Z})$ and the Hamiltonian $\hat{H}_{E1}$ be $\sum_j h_E j |j\rangle_{E\,E}\langle j|$. We define the displacement operator $V_{E1} := \sum_j |j+1\rangle_{E\,E}\langle j|$.

Definition 8 (shift-invariant unitary). A unitary U on $\mathcal{H}_I \otimes \mathcal{H}_{E1}$ is called shift-invariant when

$$UV_{E1} = V_{E1}U. \tag{26}$$

Indeed, there is a one-to-one correspondence between a shift-invariant unitary on $\mathcal{H}_I \otimes \mathcal{H}_{E1}$ and a unitary on $\mathcal{H}_I$. To give the correspondence, we define an isometry W from $\mathcal{H}_I$ to $\mathcal{H}_I \otimes \mathcal{H}_{E1}$:

$$W := \sum_x \left| -\frac{h_x}{h_E} \right\rangle_E \otimes \Pi_x. \tag{27}$$

Lemma 6. A shift-invariant unitary U is energy conserving if and only if $W^\dagger U W$ is unitary. Conversely, for a given unitary U_I on $\mathcal{H}_I$, the operator

$$F[U_I] := \sum_j V_{E1}^j W U_I W^\dagger V_{E1}^{-j} \tag{28}$$

on $\mathcal{H}_I \otimes \mathcal{H}_{E1}$ is a shift-invariant and energy-conserving unitary. Then we have

$$W^\dagger F[U_I] W = U_I. \tag{29}$$

Notice that the right-hand side of (28) is the same as the model given by Åberg [see (S9) of the Supplemental Material in [45]].

Proof. The image of W is the eigenspace of the Hamiltonian $\hat{H}_I + \hat{H}_{E1}$ associated with the eigenvalue 0. Then we denote the projection on the above space by P_0. Hence, the spectral decomposition of the Hamiltonian $\hat{H}_I + \hat{H}_{E1}$ is $\sum_j h_E j V_{E1}^j P_0 V_{E1}^{-j}$. Since the unitary satisfies the shift-invariant condition, the condition (18) is equivalent to the condition $P_0 U = P_0 U$. The latter condition holds if and only if $W^\dagger U W$ is unitary.

When U_I is a unitary on $\mathcal{H}_I$, $W U_I W^\dagger$ is a unitary on the image of W. So the operator $\sum_j V_{E1}^j W U_I W^\dagger V_{E1}^{-j}$ on $\mathcal{H}_I \otimes \mathcal{H}_{E1}$ is a shift-invariant and energy-conserving unitary. Equation (29) follows from the constructions. ■

Due to (29) in Lemma 6, we find the one-to-one correspondence between a shift-invariant unitary on $\mathcal{H}_I \otimes \mathcal{H}_{E1}$ and a unitary on $\mathcal{H}_I$. When the unitary U_I is written as $\sum_{x,x'} u_{x,x'} |x\rangle\langle x'|$, the unitary $F[U_I]$ has another expression

$$F[U_I] = \sum_{j,x,x'} u_{x,x'} |x\rangle\langle x'| \otimes \left| j + \frac{h_{x'}}{h_E} - \frac{h_x}{h_E} \right\rangle_{E\,E}\langle j|. \tag{30}$$

To consider such a case, we impose the following condition.

Definition 9 (shift-invariant FQ work extraction). We call an FQ work extraction $(\mathcal{H}_E,\hat{H}_E,U,\rho_E)$ shift invariant when the following conditions hold.

Condition 1. The external system E is the nondegenerate system $E1$, or the composite system of the nondegenerate system $E1$ and a fully degenerate system $E2$. That is, the Hamiltonian on the additional external system $E2$ is a constant.

Condition 2. The unitary U on $(\mathcal{H}_I \otimes \mathcal{H}_{E2}) \otimes \mathcal{H}_{E1}$ is shift invariant and

$$w_j = h_E j - \mathrm{Tr}\hat{H}_E\rho_E. \tag{31}$$

We can interpret the shift-invariant FQ- work extraction as the work extraction without memory effect when the external system is in the nondegenerate external system $\mathcal{H}_{E1}$. Let us consider the situation that we perform CP work extractions n times. In these applications, the state reduction of the external system $\mathcal{H}_{E1}$ is based on the projection postulate. Let $\rho_E^{(1)}$ be the initial state on the external system $\mathcal{H}_{E1}$, which is assumed to be a pure state. We assume that the initial state $\rho_E^{(k)}$ on $\mathcal{H}_{E1}$ of the kth CP work extraction is the final state of the external system of the $(k-1)$th work extraction. Other parts of the kth CP work extraction are the same as those of the first CP work extraction. Hence, the kth CP work extraction is $(\mathcal{H}_E,\hat{H}_E,\rho_E^{(k)},U)$. Generally, the FQ work extraction $(\mathcal{H}_E,\hat{H}_E,\rho_E^{(k)},U)$ depends on the state $\rho_E^{(k)}$. Namely, there exists a memory effect. However, when U is shift invariant, the FQ work extraction does not depend on the state $\rho_E^{(k)}$. Then the memory effect does not exist. So we do not have to initialize the external system after the projective measurement on the external system.

Then the shift-invariant FQ work extraction can simulate the semiclassical scenario in the following limited sense.

Lemma 7. Given an internal unitary U_I and a state ρ_I of the internal system I, in the shift-invariant FQ work extraction $\mathcal{F} = (\mathcal{H}_E,\hat{H}_E,F[U_I],\rho_E)$ and the average amount of extracted work is $\mathrm{Tr}\rho_I\hat{H}_I - \mathrm{Tr}U_I\rho U_I^\dagger\hat{H}_I$.

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

Lemma 8. For an energy-conserving and shift-invariant FQ work extraction $\mathcal{F} = (\mathcal{H}_E,\hat{H}_E,U,\rho_E)$, the CP work extraction CP($\mathcal{F}$) satisfies the level-3 energy-conservation law.

Proof. First, we consider the case when $\mathcal{H}_E = \mathcal{H}_{E1}$. Similar to the proof of Lemma 3, we have

$$\begin{aligned}
P_{KY|X}(k,y|x) =& \sum_{j:h_x-h_y-w_j=k} \mathrm{Tr}U(\Pi_x\otimes\rho_E)U^\dagger(\Pi_y\otimes|j\rangle\langle j|)\\
=& \sum_{j:h_x-h_y-w_j=k} \mathrm{Tr}U(\Pi_x\otimes\rho_E)U^\dagger(\Pi_y\otimes|j\rangle\langle j|^2)\\
\overset{(a)}{=}& \sum_{j':h_E j'=-k+\mathrm{Tr}\hat{H}_E\rho_E} \mathrm{Tr}[U(\Pi_x\otimes|j'\rangle\langle j'|\rho_E|j'\rangle\langle j'|)U^\dagger(\Pi_y\otimes\hat{1}_E)]\\
=&|\langle y|U_I|x\rangle|^2 \sum_{j':h_E j'=-k+\mathrm{Tr}\hat{H}_E\rho_E} \langle j'|\rho_E|j'\rangle,
\end{aligned} \tag{32}$$

where (a) can be shown by using relations similar to (21) and (22). Hence,

$$P_{K|Y,X}(k|y,x) = \sum_{j':h_E j'=-k+\mathrm{Tr}\hat{H}_E\rho_E} \langle j'|\rho_E|j'\rangle, \tag{33}$$

which does not depend on x or y.

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

$$\begin{aligned}
P_{KY|X}(k,y|x) =& \sum_{j:h_x-h_y-w_j=k} \mathrm{Tr}U(\Pi_x\otimes\rho_{E2}\otimes\rho_{E1})U^\dagger(\Pi_y\otimes\hat{1}_{E2}\otimes|j\rangle\langle j|)\\
=& (\mathrm{Tr}U_I\Pi_x\otimes\rho_{E2}U_I^\dagger\Pi_y\otimes\hat{1}_{E2}) \sum_{j':h_E j'=-k+\mathrm{Tr}\hat{H}_E\rho_E} \langle j'|\rho_E|j'\rangle.
\end{aligned} \tag{34}$$

Hence, we obtain (33). ■

As a special case of Theorem 1, we have the following lemma.

Lemma 9. Let $\mathcal{F} = (\mathcal{H}_E,\hat{H}_E,U,\rho_E)$ be an energy-conserving and shift-invariant FQ work extraction. Then the support of the initial state ρ_E belongs to an eigenspace of the Hamiltonian $\hat{H}_E$ if and only if the CP work extraction CP($\mathcal{F}$) satisfies the level-4 energy-conservation law.

Lemma 10. For a level-4 CP work extraction $\{\mathcal{E}_j,w_j\}_{j\in\mathcal{J}}$, there exists an energy-conserving and shift-invariant FQ work extraction $\mathcal{F}$ such that the support of the initial state ρ_E belongs to an eigenspace of the Hamiltonian $\hat{H}_E$ and CP($\mathcal{F}$) $= \{\mathcal{E}_j,w_j\}_{j\in\mathcal{J}}$.

Proof. We make a Stinespring extension $(\mathcal{H}_{E2},U_{IE2},\rho_{E2})$ with a projection-valued measure $\{E_j\}$ on $\mathcal{H}_{E2}$ of $\{\mathcal{E}_j,w_j\}_{j\in\mathcal{J}}$ as follows:

$$\mathcal{E}_j(\rho_I) = \mathrm{Tr}_{E2}U_{IE2}(\rho_I\otimes\rho_{E2})U_{IE2}^\dagger(\hat{1}_I\otimes E_j), \tag{35}$$

where $\{E_j\}$ is a projection-valued measure on $\mathcal{H}_{E2}$ and ρ_E is a pure state. This extension is often called the indirect measurement model, which was introduced by Ozawa [52]. Here the Hamiltonian of $\mathcal{H}_{E2}$ is chosen to be 0. Next we define the unitary U on $\mathcal{H}_I \otimes \mathcal{H}_{E2} \otimes \mathcal{H}_{E1}$ as $U = F[U_{IE2}]$. Here $\mathcal{H}_{E1}$ is defined as in the above discussion.

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

$$\mathcal{E}_j(\rho) = \mathrm{Tr}_E U(\rho_I \otimes |0\rangle\langle 0| \otimes \rho_{E2}) U^\dagger (\hat{1}_{IE2} \otimes \Pi_j). \quad (36)$$

■

It is natural to consider that the state on the additional external system $E2$ does not change due to the work extraction. Hence, we impose the following restriction for the state on the additional external system $E2$.

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

$$\mathrm{Tr}_{IE1} U(\rho_I \otimes \rho_E) U^\dagger = \rho_{E2} \quad (37)$$

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

Now we have the following theorem.

Theorem 2. Let $\mathcal{F} = (\mathcal{H}_E, \hat{H}_E, U, \rho_E)$ be a stationary FQ work extraction. Then the CP work extraction $CP(\mathcal{F})$ satisfies the unital condition (13).

Proof. First, we consider the case when $\mathcal{H}_E = \mathcal{H}_{E1}$. To show the unital condition (13), it is enough to show that

$$\mathrm{Tr}_I |\psi_I\rangle\langle\psi_I| \mathrm{Tr}_E U(I \otimes \rho_E) U^\dagger = 1 \quad (38)$$

for any pure state $|\psi_I\rangle$ on $\mathcal{H}_I$. The shift-invariant property (C1) implies that

$$\begin{aligned}\langle y, j'|U|x, j\rangle &= \langle y, j'|U V_{E1}^{j+j'}|x, -j'\rangle \\ &= \langle y, j'|V_{E1}^{j+j'} U|x, -j'\rangle \\ &= \langle y, -j|U|x, -j'\rangle. \end{aligned} \quad (39)$$

When $\rho_E = |\psi_E\rangle\langle\psi_E|$, $|\psi_E\rangle = \sum_j b_j |j\rangle$, and $|\psi_I\rangle = \sum_x a_x |x\rangle$, we have [55]

$$\begin{aligned}&\mathrm{Tr}_I |\psi_I\rangle\langle\psi_I| \mathrm{Tr}_E U(I \otimes \rho_E) U \\ &= \sum_{x,j} |\langle\psi_I, j|U|x, \psi_E\rangle|^2 \\ &= \sum_{x,j'} \left| \sum_y \bar{a_y} \sum_j b_j \langle y, j'|U|x, j\rangle \right|^2 \\ &= \sum_{x,j'} \left| \sum_y \bar{a_y} \sum_j b_j \langle y, -j|U|x, -j'\rangle \right|^2 \\ &= \sum_y \bar{a_y} \sum_j b_j \sum_{\tilde{y}} \bar{a_{\tilde{y}}} \sum_{\tilde{j}} b_{\tilde{j}} \langle y, -j|y, -\tilde{j}\rangle \\ &= \sum_y |\bar{a_y}|^2 \sum_j |b_j|^2 = 1. \end{aligned} \quad (40)$$

Hence, when $\rho_E = \sum_l p_l |\psi_{E,l}\rangle\langle\psi_{E,l}|$, we also have

$$\mathrm{Tr}_I |\psi_I\rangle\langle\psi_I| \mathrm{Tr}_E U(I \otimes \rho_E) U = 1. \quad (41)$$

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

$$\mathrm{Tr}_{E1} U\left(\frac{\hat{1}_I}{d_I} \otimes \frac{\hat{1}_{E2}}{d_{E2}} \otimes \rho_{E1}\right) U^\dagger = \frac{\hat{1}_I}{d_I} \otimes \frac{\hat{1}_{E2}}{d_{E2}}. \quad (42)$$

The information processing inequality yields that

$$\begin{aligned}&D\left(\frac{\hat{1}_I}{d_I} \otimes \rho_{E2} \middle\| \frac{\hat{1}_I}{d_I} \otimes \frac{\hat{1}_{E2}}{d_{E2}}\right) \\ &\geqslant D\left(\mathrm{Tr}_{E1} U\left(\frac{\hat{1}_I}{d_I} \otimes \rho_{E2} \otimes \rho_{E1}\right) U^\dagger \right\| \\ &\quad \times \mathrm{Tr}_{E1} U\left(\frac{\hat{1}_I}{d_I} \otimes \frac{\hat{1}_{E2}}{d_{E2}} \otimes \rho_{E1}\right) U^\dagger \Big) \\ &\geqslant D\left(\mathrm{Tr}_{E1} U\left(\frac{\hat{1}_I}{d_I} \otimes \rho_{E2} \otimes \rho_{E1}\right) U^\dagger \middle\| \frac{\hat{1}_I}{d_I} \otimes \frac{\hat{1}_{E2}}{d_{E2}}\right), \end{aligned} \quad (43)$$

which implies that

$$S\left(\mathrm{Tr}_{E1} U\left(\frac{\hat{1}_I}{d_I} \otimes \rho_{E2} \otimes \rho_{E1}\right) U^\dagger\right) \geqslant \log d_I + S(\rho_{E2}). \quad (44)$$

Due to the condition (37), the reduced density operator $\mathrm{Tr}_{E1} U(\frac{\hat{1}_I}{d_I} \otimes \rho_{E2} \otimes \rho_{E1}) U^\dagger$ on $E2$ is ρ_{E2}. Under this condition, we have the inequality (44). The equality in (44) holds only when $\mathrm{Tr}_{E1} U(\frac{\hat{1}_I}{d_I} \otimes \rho_{E2} \otimes \rho_{E1}) U^\dagger = \frac{\hat{1}_I}{d_I} \otimes \rho_{E2}$, which implies the unital condition (13). ■

Overall, as a realizable heat engine, we impose the energy-conserving, shift-invariant, and stationary conditions to our FQ work extractions. Also, it is natural to assume that the initial state on $E1$ is an eigenstate of the Hamiltonian $\hat{H}_{E1}$ because it is not easy to prepare a noneigenstate of the Hamiltonian $\hat{H}_{E1}$. Namely, we define the standard FQ work extraction as follows.

Definition 11. When an FQ work extraction satisfies the energy-conserving, shift-invariant, stationary conditions and the condition that the initial state on $E1$ is an eigenstate of the Hamiltonian $\hat{H}_{E1}$, we refer to it as a standard FQ work extraction.

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

However, we can consider restricted classes of standard FQ work extractions by considering additional properties. For a standard FQ work extraction $\mathcal{F} = (\mathcal{H}_E, \hat{H}_E, U, \rho_E)$, we assume that the external system $\mathcal{H}_E$ consists only of a nondegenerate external system $\mathcal{H}_{E1}$. In this case, the corresponding standard CP work extraction CP($\mathcal{F}$) depends only on the internal unitary $U_I = WUW^\dagger$.

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

Further, an internal unitary U_I is called deterministic when $\langle x|U_I|x'\rangle$ is zero or $e^{i\theta}$ for any x and x'. In the latter, a standard

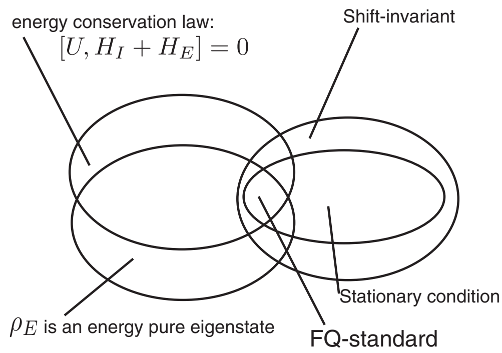

FIG. 6. Venn diagram of the FQ work extractions.

CP work extraction associated with the deterministic internal unitary plays an important role.

We illustrate a Venn diagram of the FQ work extractions in Fig. 6 and classify the relationships among the classes of the CP work extraction and that of the FQ work extraction in Table I.

Finally, we consider the relation with the classical standard formulation. In the shift-invariant unitary, if we focus on the eigenstates, the state $|i,j\rangle$ can be regarded as being probabilistically changed to $|i',j'\rangle$ with the energy-conserving law

$$h_i + h_E j = h_{i'} + h_E j', \tag{45}$$

which is the same as in the classical standard formulation. When we focus on the internal system, $|i\rangle$ is changed to $|i'\rangle$. So in the semiclassical scenario, they make a unitary time evolution based on the states on the internal system. However, the time evolution occurs between the internal and external systems as $|i,j\rangle \mapsto |i',j'\rangle$ in the classical standard formulation under the condition (45). So to consider its natural quantum extension, we need to make a unitary evolution on the composite system. That is, it is natural to add proper complex amplitudes to the time evolution $|i,j\rangle \mapsto |i',j'\rangle$ so that it forms a unitary evolution on the composite system. Hence, our shift-invariant unitary can be regarded as a natural quantum extension of the classical standard formulation because it is constructed in this way.

One might consider that there is a cost for initialization of the measurement. However, if we adopt the projection postulate, this problem can be resolved when we employ a shift-invariant model. The classical standard formulation does not describe the dynamics of the external system, explicitly because the dynamics of the internal system does not depend on the state of the external system. Similarly, under our shift-invariant model, the dynamics of the internal system does not depend on the state of the external system as long as the initial state of the external system is an energy eigenstate. When the projection postulate holds for our measurement, the final state of the external system is an energy eigenstate, which can be used as the initial state for the next work extraction. In real systems, decoherence occurs during unitary evolution such that the state of the external system becomes inevitably an energy eigenstate.

Further, we should notice that the initialization of the measurement is different from the initialization of the thermal bath. In the finite-size setting, the final state in the thermal bath is different from the thermal state in general. Hence, we need to consider the initialization of the thermal bath. However, the thermal bath is considered as a part of the internal system in our model. So this problem is different from the initialization of the measurement and will be discussed in [56].

Although we consider only the lattice case, in real systems, there are so many cases with a nonlattice Hamiltonian. Our discussion can be extended to the nonlattice case with a small modification. Details are given in Appendix C.

V. TRADE-OFF BETWEEN INFORMATION LOSS AND COHERENCE

A. Approximation and coherence

In this section we investigate the validity of the semiclassical scenario [21–34] based on an FQ work-extraction model. To discuss this issue, we first recall the semiclassical scenario as follows. We consider that to extract work, an external agent performs the external operation as the unitary time evolution $U_I := \mathcal{T}\{\exp[\int -i\hat{H}_I(t)dt]\}$ [$\mathcal{T}(\cdots)$ denotes the time-ordered product] on I by time-dependently varying the control parameter of the Hamiltonian $\hat{H}_I(t)$ of the internal system I, which usually consists of the system S and the heat bath B. During the time evolution, the loss of energy of the internal system is transmitted to the external controller through the backreaction of the control parameter. So the energy loss is regarded as the extracted work (see Sec. 2 in [21]). This scenario is considered as a natural quantum extension of the classical standard formulation [7].

In the semiclassical scenario, it is expected that the unitary can be realized via the control of the Hamiltonian of the internal system. Since the control is realized by the external system, we consider that the work can be transferred to the external

TABLE I. Correspondence between FQ work extraction and CP work extraction, describing the type of CP work extraction that can be generated by respective classes of FQ work extraction.

CP($\mathcal{F}$)	FQ energy conservation, ρ_E is not an energy eigenstate	FQ energy conservation, shift invariant	Stationary condition	FQ energy conservation, ρ_E is an energy eigenstate
CP level 2	yes (Lemma 3)	yes		yes
CP level 3		yes (Lemma 4)		yes
CP level 4	no (Theorem 1)			yes (Theorem 1)
CP unital			yes (Theorem 2)	

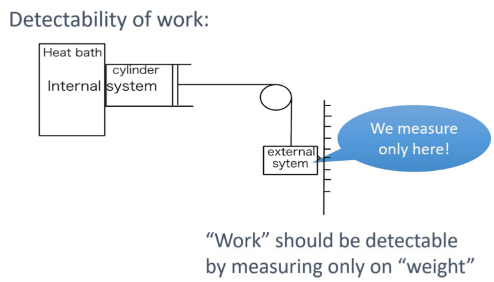

FIG. 7. Concepts of the detectability of work.

system via the control. In this scenario, we expect that the time evolution Λ of the internal system $\mathcal{H}_I$ can be approximated to an ideal unitary U_I. That is, when we employ an FQ work extraction $\mathcal{F} = (\mathcal{H}_E, \hat{H}_E, U, \rho_E)$, the time evolution Λ of the internal system $\mathcal{H}_I$ is given as $\Lambda(\rho_I) = \mathrm{Tr}_E U(\rho_I \otimes \rho_E)U^\dagger$. To qualify the approximation to the unitary U_I, we need to focus on two aspects. One is the time evolution of basis states in a basis $\{|x\rangle\}_x$ diagonalizing the Hamiltonian $\hat{H}_I$. The other is the time evolution of superpositions of states in this basis. Usually, it is not difficult to realize the same evolution as that of U_I only for the former states. However, it is not easy to keep the quality of the latter time evolution, which is often called the coherence. Hence, we fix a unitary U_I and we assume that the CPTP map Λ satisfies the condition

$$\langle y|\Lambda(|x\rangle\langle x|)|y\rangle = \langle y|U_I|x\rangle\langle x|U_I^\dagger|y\rangle \quad \text{for any } x,y. \tag{46}$$

That is, we choose our time evolution among CPTP maps satisfying the above condition. Under the condition, the quality of the approximation to the unitary U_I can be measured by the coherence of the CPTP map Λ. For a measure of coherence, we employ the entropy exchange [57]

$$S_e(\Lambda, \rho_I) := S(\Lambda(|\Phi\rangle\langle\Phi|)), \tag{47}$$

where $|\Phi\rangle$ is the purification of the state ρ_I with the reference system R. When a CPTP map Λ satisfies (46) and $S_e(\Lambda,\rho_I) \ll 1$, we say that $\Lambda \approx U_I$.

B. Expression of detectability of work in terms of correlation

On the other hand, we need to focus on another feature of thermodynamics, i.e., the detectability of work (Fig. 7). In standard thermodynamics, we can measure the amount of extracted work by measuring only the work storage system, e.g., the weight. In order that the heat engine works properly as energy transfer from a collection of microscopic systems to a macroscopic system, the amount of extracted work needs to be reflected to the outer system that consists of the macroscopic devices. Hence, the amount of energy loss in the internal system is required to be correlated to the outer system. So we can measure the detectability of work by the correlation between the external system E after energy extraction and the energy loss in the internal system I. In Fig. 8 the former is expressed as A and the latter as B. Our purpose in this section is to show a trade-off relation, which indicates the impossibility of the detection of work under the condition $\Lambda \approx U_I$. Namely, when $\Lambda \approx U_I$, the correlation between A and B in Fig. 8 is close to zero.

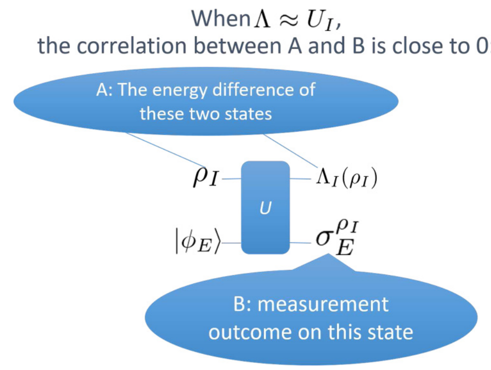

FIG. 8. Concept of our trade-off relation. Here $\sigma_E^{\rho_I} := \mathrm{Tr}_I[U(\rho_I \otimes |\phi\rangle\langle\phi|_E)U^\dagger]$.

In order to show the trade-off relation, we employ the purification $|\Phi\rangle$ of the state ρ_I with the reference system R, which satisfies $\mathrm{Tr}_I[|\Phi\rangle\langle\Phi|] = \mathrm{Tr}_E[|\Phi\rangle\langle\Phi|] = \rho_I$. Then we can interpret R as a kind of memory and translate the energy loss of I during the time evolution Λ into the energy difference between I and R after the time evolution (Fig. 9). We also employ the initial state ρ_E on the external system E. Here we take the external system to be large so that the time evolution on the joint system of I and E can be regarded as a unitary U on IE and the state ρ_E is a pure state $|\phi_E\rangle$. In the following, we denote the initial state $|\Phi,\phi_E\rangle\langle\Phi,\phi_E|$ of the total system $\mathcal{H}_I \otimes \mathcal{H}_R \otimes \mathcal{H}_E$ by ρ_{IRE}. Then we denote the resultant state $U|\Phi,\phi_E\rangle\langle\Phi,\phi_E|U^\dagger$ by ρ'_{IRE}.

To determine the amount of energy lost from the internal system, we consider a measurement of the observable $\hat{H}_I - \hat{H}_R$ on the joint system I and R after the time evolution Λ (Fig. 10). That is, by using the spectral decomposition $\hat{H}_I - \hat{H}_R = \sum_z zF_z$, we define the final state ρ''_{ZE} on $\mathcal{H}_Z \otimes \mathcal{H}_E$ by

$$\rho''_{ZE} := \sum_z |z\rangle_{Z\,Z}\langle z| \otimes \mathrm{Tr}_{IR} F_z \rho'_{IRE}. \tag{48}$$

Here the random variable Z takes the value z with probability $P_Z(z) := \mathrm{Tr}\rho'_{IRE}F_z = \mathrm{Tr}\Lambda(|\Phi\rangle\langle\Phi|)F_z$. When the outcome Z is z, the resultant state on E is $\rho''_{E|Z=z} := \frac{1}{P_Z(z)}\mathrm{Tr}_{IR}\rho'_{IRE}F_z$. So the correlation between the external system E and the amount of energy loss can be measured by the correlation on the state $\rho_{Z,E}$. Although this scenario is based on a virtual measurement, this interpretation will be justified by considering the situation without the purification in the following lemma.

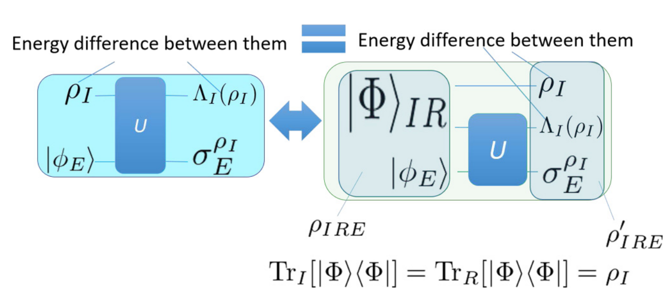

FIG. 9. We can translate the energy loss of I during the time evolution Λ into the energy difference between I and R.

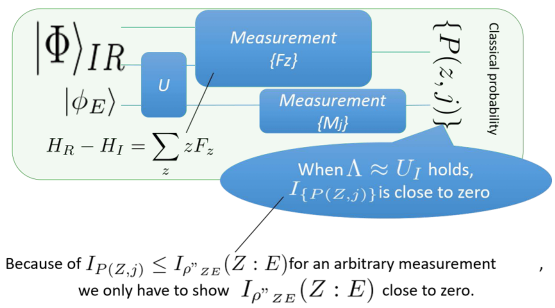

FIG. 10. Schematic diagram of the formulation.

Lemma 11. We consider the case when the eigenstate $|\psi_{I,a}\rangle$ is generated with probability $P_A(a)$. Measuring the Hamiltonian $\hat{H}_I = \sum_h hP_h$ after the time evolution Λ, we obtain the conditional distribution $P_{H|A}(h|a) := \mathrm{Tr} P_h \Lambda(|\psi_{I,a}\rangle\langle\psi_{I,a}|)$. Then we choose the state ρ_I to be

$$\rho_I = \sum_a P_A(a)|\psi_{I,a}\rangle\langle\psi_{I,a}|. \tag{49}$$

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

$$\sum_{h,a:\langle\psi_{I,a}|\hat{H}_I|\psi_{I,a}\rangle - h = z} P_{HA}(h,a) = P_Z(z). \tag{50}$$

Since the proof of Lemma 11 is trivial, we skip its proof. Lemma 11 guarantees that the probability distribution $P_Z(z)$ is the same as the work distribution defined in [33] under its assumption. When ρ_I commutes with $\hat{H}_I$, we can take the above eigenstate $|\psi_{I,a}\rangle$ and a probability distribution P_A satisfying the above condition (49). Also, when the state ρ_I is a Gibbs state or a mixture of Gibbs states, the state ρ_I satisfies the condition in Lemma 11. Hence, it is suitable to consider the distribution P_Z of the amount of energy lost in this case.

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

$$\begin{aligned} I_{\rho''_{ZE}}(Z;E) &:= D(\rho''_{ZE}\|\rho''_Z \otimes \rho''_E) \\ &= S(\rho''_E) - \sum_z P_Z(z)S(\rho''_{E|Z=z}) \overset{(a)}{\geqslant} S(\rho''_E) \\ &= S(\Lambda(|\Phi\rangle\langle\Phi|)), \end{aligned} \tag{51}$$

where $D(\tau\|\sigma) := \mathrm{Tr}\tau(\log\tau - \log\sigma)$. Here the equality in (a) holds if and only if the state $\rho''_{E|Z=z}$ is pure for any value z with nonzero probability $P_Z(z)$. The information processing inequality for the map $|z\rangle\langle z| \mapsto \rho''_{E|Z=z}$ yields

$$I_{\rho''_{ZE}}(Z;E) \leqslant S(P_Z). \tag{52}$$

In particular, the equality in (52) holds in the ideal case, i.e., in the case when the states $\{\rho''_{E|Z=z}\}_z$ are distinguishable, i.e., $\mathrm{Tr}\rho''_{E|Z=z}\rho''_{E|Z=z'} = 0$ for $z \neq z'$ with nonzero probabilities $P_Z(z)$ and $P_Z(z')$. For example, when U satisfies the energy-conservation law (18), the initial state of the internal system commutes with the internal Hamiltonian $\hat{H}_I$, and the initial state of the external system is an energy eigenstate, this conditions holds because the energy of the final state of the external system precisely reflects the loss of energy of the internal system. So the imperfectness of the correlation for the decrease of the energy can be measured by the difference

$$\Delta I_{\rho''_{ZE}}(Z;E) := S(P_Z) - I_{\rho''_{ZE}}(Z;E). \tag{53}$$

C. Trade-off with imperfection of correlation

Many papers studied trade-off relations between the approximation of a pure state on the bipartite system and the correlation with the third party E. In particular, since this kind of relation plays an important role in the security analysis in a quantum key distribution (QKD), it has been studied mainly by several researchers in a QKD and related areas with various formulations [see, e.g., Sec. V C in [57], (21) in [58], Theorem 1 in [59], Lemma 2 in [60], Theorem 2 in [61], and [62,63]].

However, these trade-off relations are not suitable for our situation. So we derive two kinds of trade-off relations with the imperfectness of correlation, which are more suitable for our purpose.

Theorem 3. The amount of decoherence $S_e(\Lambda,\rho_I)$ and the amount of imperfectness of correlation $\Delta I_{\rho''_{ZE}}(Z;E)$ satisfy the following trade-off relation:

$$S_e(\Lambda,\rho_I) + \Delta I_{\rho''_{ZE}}(Z;E) \geqslant S(P_Z). \tag{54}$$

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

$$S_e(\Lambda,\rho_I) = I_{\rho''_{ZE}}(Z;E) = S\left(\sum_z P_Z(z)|\psi_{E|Z=z}\rangle\langle\psi_{E|Z=z}|\right). \tag{55}$$

Proof. Since (51), (47), and (53) imply

$$\begin{aligned} S_e(\Lambda,\rho_I) + \Delta I_{\rho''_{ZE}}(Z;E) &= S(P_Z) - I_{\rho''_{ZE}}(Z;E) + S(\rho''_E) \\ &= S(P_Z) + \sum_z P_Z(z)S(\rho''_{E|Z=z}) \\ &\geqslant S(P_Z), \end{aligned} \tag{56}$$

the equality holds if and only if the state $\rho''_{E|Z=z}$ is pure for any value z with nonzero probability $P_Z(z)$. In this case, we have $\rho''_E = \sum_z P_Z(z)|\psi_{E|Z=z}\rangle\langle\psi_{E|Z=z}|$, which implies (55). ■

Due to the relation (54), when the imperfectness $\Delta I_{\rho''_{ZE}}(Z;E)$ of the correlation is close to zero, the amount of decoherence $S_e(\Lambda,\rho_I)$ is far from zero. So the coherence cannot be kept in this work-extraction process. That is, the unitary U_I cannot be approximated by the actual time evolution Λ. On the other hand, when the amount of decoherence $S_e(\Lambda,\rho_I)$ is close to zero, the imperfectness $\Delta I_{\rho''_{ZE}}(Z;E)$ of the correlation is far from zero. In this case, the perfect approximation is realized although the external system has almost no correlation.

In the current discussion, we deal with a general framework for the ensemble of initial states of the internal system. In practice, it is quite difficult to realize an arbitrary distribution of the initial state. However, without requiring the realization of an arbitrary distribution, we have a realistic example to derive a contradiction for the semiclassical model. That is, in such a desired example, if the coherence is kept, which is the requirement of the semiclassical model, we cannot detect the amount of extracted work precisely. To give such an example, it is sufficient to consider an ensemble whose entropy is greater than $\log 2$. For example, a useful internal state (in which work extraction is possible) occurs with probability $\frac{1}{2}$ and a useless internal state (in which work extraction is impossible) occurs with probability $\frac{1}{2}$, i.e., with probability $\frac{1}{2}$, we cannot extract work from the initial state. In this example, when the amount of decoherence $S_e(\Lambda,\rho_I)$ is close to zero, the imperfectness $\Delta I_{\rho''_{ZE}}(Z;E)$ of the detection of the amount of extracted work is close to $\log 2$, which is far from zero. Since such an ensemble is possible in the real world, this example shows that the semiclassical model is not suitable for the model of a heat engine because we cannot detect the amount of extracted work precisely.

D. Shift-invariant model

Next we consider how to realize the case when the amount of decoherence $S_e(\Lambda,\rho_I)$ is close to zero. The following theorem is the solution to this problem, which will be shown in Appendix B 4.

Theorem 4. We assume the shift-invariant model without an additional external system. When

$$|\psi_E\rangle = \sum_j \sqrt{P_J(j)}|j\rangle, \tag{57}$$

$$P_J(j) = \begin{cases} \frac{1}{2m+1} & \text{if } |j| \leqslant m \\ 0 & \text{otherwise,} \end{cases} \tag{58}$$

$$P_Z(h_E j) = 0 \quad \text{if } |j| \geqslant l, \tag{59}$$

we have

$$S_e(\Lambda,\rho_I) \leqslant h\left[2\frac{l}{2m+1} - \left(\frac{l}{2m+1}\right)^2\right] + \left[2\frac{l}{2m+1} - \left(\frac{l}{2m+1}\right)^2\right]\log\left(d_I^2 - 1\right). \tag{60}$$

So when m is sufficiently large, the quality of approximation is very small under the shift-invariant model without an additional external system. That is, a large superposition enables us to keep coherence. This consequence is qualitatively consistent with the conclusion in [45] (see Proposition 2 of the Supplemental Material therein), which assesses the quality of the approximation with the trace norm unlike Theorem 4.

E. Trade-off under CP work extraction

In Sec. V C we discussed the trade-off relation between the imperfectness of correlation and the quality of approximation under an FQ work extraction. In this section we discuss the trade-off relation under a CP work extraction $\mathcal{G} := \{\mathcal{E}_j, w_j\}_j$ on the internal system $\mathcal{H}_I$ with the Hamiltonian $\hat{H}_I$. To discuss the trade-off relation, in the internal system $\mathcal{H}_I$, we consider the internal unitary U_I to be approximated and the initial mixed state ρ_I is assumed to commute with $\hat{H}_I$. To quantify the approximation, we employ the measure $S_e(\sum_j \mathcal{E}_j,\rho_I)$. To evaluate the imperfectness of correlation, we consider the purification $|\Phi\rangle$ of ρ_I and introduce the joint distribution P_{ZW} as

$$P_{ZW}(z,w) := \sum_{j:w_j=w} \mathrm{Tr}_{RI}\mathcal{E}_j(|\Phi\rangle\langle\Phi|)F_z, \tag{61}$$

where the projection F_z is defined in the same way as in Sec. V B. Then we employ the measure $\Delta I_{P_{ZW}}(Z;W) := S(P_Z) - I_{P_{ZW}}(Z;W)$. Since the measurement outcome precisely reflects the decrease in energy of the internal system in a level-4 energy CP work extraction $\{\mathcal{E}_j,w_j\}_j$, we have the following lemma.

Lemma 12. For a level-4 energy CP work extraction $\{\mathcal{E}_j,w_j\}_j$, the relation $\Delta I_{P_{ZE}}(Z;E) = 0$ holds for any internal state ρ_I that commutes with $\hat{H}_I$.

This lemma shows that a level-4 energy CP work extraction satisfies our requirement explained in the Introduction. As a corollary of Theorem 3 we have the following, by virtually considering the indirect measurement.

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

$$S_e\left(\sum_j \mathcal{E}_j,\rho_I\right) + \Delta I_{P_{ZW}}(Z;W) \geqslant S(P_Z). \tag{62}$$

Proof. Notice that Theorem 3 does not assume any energy-conservation law. Then we take a Stinespring representation $(\mathcal{H}_E,U,\rho_E)$ with a pure state ρ_E of $\{\mathcal{E}_j,w_j\}_{j\in\mathcal{J}}$ as follows:

$$\mathcal{E}_j(\rho_I) = \mathrm{Tr}_E U_{IE}(\rho_I\otimes\rho_E)U_{IE}^{\dagger}(\hat{1}_I\otimes E_j), \tag{63}$$

where $\{E_j\}$ is a projection-valued measure on $\mathcal{H}_E$. Notice that $(\mathcal{H}_E,U,\rho_E)$ is an FQ work extraction. Here we do not care whether the FQ work extraction satisfies any energy-conservation law. Then we apply Theorem 3. Since the information processing inequality for the relative entropy yields $I_{\rho''_{ZE}}(Z;E) \geqslant I_{P_{ZE}}(Z;E)$, the relation (54) implies (62). ■

Further, we have the following corollary.

Corollary 2. When $\Delta I_{P_{ZE}}(Z;E) = 0$, we have

$$S_e\left(\sum_j \mathcal{E}_j,\rho_I\right) \geqslant S(P_Z). \tag{64}$$

The combination of this corollary and Lemma 12 shows that the dynamics of a level-4 CP work extraction is far from any internal unitary.

VI. OTHER CONSEQUENCES OF OUR FORMULATION AND RELATION TO OTHER FORMULATION

Finally, we discuss the relation to other formulations. While we have introduced four kinds of energy-conservation laws for measurement-based work extraction, a level-1 CP work extraction can be mathematically regarded as an average work extraction [35] as follows. In Sec. II A 2 in [64] we formulated the average work extraction by using the CPTP map on the internal system in an implicit treatment of the external work storage. For a given level-1 CP work extraction $\{\mathcal{E}_j,w_j\}_{j\in\mathcal{J}}$, we define a CPTP map $\sum_j \mathcal{E}_j$, which gives an average work extraction with implicit treatment of the external work storage. Hence, any level-1 CP work extraction can be treated as an average work extraction. Thus, any model in our paper is mathematically a part of average work extraction with implicit treatment of the external work storage. Since the optimal efficiency of an average work extraction asymptotically equals the Carnot efficiency [36,43,64], the efficiency of any our model does not exceed the Carnot efficiency.

Now we discuss the detailed relation with existing models. While our measurement-based model for work extraction treats energy transfer from a collection of microscopic systems to a macroscopic system, our model can treat energy transfer in the microscopic scale as follows. As shown in Lemma 10, a level-4 CP work extraction can be extended to an energy-conserving and shift-invariant FQ work extraction, which is the same as in [45]. Conversely, as shown in Lemma 3, an energy-conserving FQ work extraction can be converted to a level-2 CP work extraction. In particular, the combination of Theorem 1 and Lemma 10 shows that a shift-invariant model up to the second order with an initial energy eigenstate ρ_E on the external system is equivalent to a level-4 CP work extraction.

Another paper by the present authors [64] derives the higher-order expansion of the optimal efficiency under average work extraction with implicit treatment of the external work storage while its first order equals the Carnot efficiency. Furthermore, it was shown that the optimal efficiency can be attained by a shift-invariant model with an initial energy eigenstate ρ_E on the external system up to second order. In summary, even in any of our four models, the optimal efficiency asymptotically has the same value up to higher order, whereas the first-order coefficient is the Carnot efficiency. This fact shows the adequacy of our models.

As another problem one might consider a serious increase of the entropy due to the measurement. However, the increase is not so serious as follows. In Sec. 4 of Ref. [64] it is shown that we can give a concrete protocol that extracts energy with a negligibly small increase of entropy, while the protocol attains the optimal efficiency. In Sec. 4 of Ref. [64] we translate the implicit formulation of an average work extraction into the explicit formulation with an external work storage by using the translation between the direct measurement and the indirect measurement. Then we calculate the ratio of the energy gain to the entropy gain in the external work storage and show that the entropy-energy ratio of the work storage goes to 0 in the macroscopic limit.

VII. CONCLUSION

In the present article, to expand the area of quantum thermodynamics, we have discussed quantum heat engines as work-extraction processes in terms of quantum measurement. That is, we have formulated work extraction as a CP instrument when discernible energy is transferred from a collection of quantum systems to a macroscopic system. Our formulation is so general as to include any work extraction that has equipment to assess the amount of the extracted work when we extract energy to a macroscopic system. We also have clarified the relationships between the fully quantum work extraction and the CP work extraction in our context.

Moreover, to clarify the problem in the semiclassical scenario, we have given a trade-off relation for the coherence and information acquisition for the amount of extracted work. The trade-off relation means that we have to demolish the coherence of the thermodynamic system in order to know the amount of extracted energy. Further, we have pointed out that our shift-invariant unitary is a natural quantum extension of the classical standard formulation rather than the semiclassical scenario at the end of Sec. IV. In summary, these results imply the incompatibility of the coherence of the internal system and information acquisition for the amount of extracted work. That is, when the time evolution of the internal system is close to unitary, we cannot know the amount of extracted work.

In the Appendixes we also show the reduction to the classical model. When the initial state of the internal system commutes with the Hamiltonian, any CP work extraction can be simulated by a classical work extraction in the nonasymptotic sense, whose detailed definition is shown in the Appendixes. This conversion is helpful for analyzing the performance of the work-extraction process. This property is employed for derivation of optimal efficiency with the asymptotic setting in another paper [64].

A reader might raise the following question for our formulation as follows. Although this paper requires the distinguishability of the amount of extracted work, it is sufficient to recover this property only within the thermodynamic limit because the identification of the amount of extracted work is a classical task. Hence, we do not need to employ measurement to formulate the quantum heat engine. However, this idea is not correct for the following two reasons when we extract energy from a collection of microscopic system to a macroscopic system.

First, our trade-off relation between the coherence and the distinguishability holds independently of the size of the system. So even though we take the thermodynamic limit, we cannot resolve this trade-off. So to keep the distinguishability of the amount of extracted work even with the thermodynamic limit, we need to give up the description by the internal unitary. Second, to avoid the distinguishability, we can employ a scenario that the extracted work is autonomously stored in a quantum storage [35–42,65,66]. (The word "autonomous" is used in Refs. [65,66], for example.) This scenario works well when we extract energy from a microscopic system to another microscopic system. However, when we extract energy from a collection of microscopic systems to a macroscopic system, even in this scenario, we ultimately consume the work stored in the quantum storage. In the consuming stage, we have to consider the distinguishability of the amount of work extracted from the quantum storage. Therefore, we cannot avoid distinguishing the amount of extracted work. That is, the solution depends on the situation and the measurement is inevitably essential for a proper formulation of the quantum heat engine in our situation.

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APPENDIX A: ORGANIZATION OF THE APPENDIXES

Before starting proceeding, we briefly explain the organization of the Appendixes. In Appendix B we give a discussion similar to Sec. V based on the fidelity instead of the entropic quantity. Although the fidelity requires a more complicated discussion, it provides tighter evaluation for the coherence of the dynamics. Further, using the discussion based on the fidelity, we give a proof of Theorem 4. Since this discussion needs several technical lemmas, they are given in Appendix E.

In Appendix C we extend the discussion for the shift-invariant model in Sec. IV to the case with a nonlattice Hamiltonian. In Appendix D we discuss the relation between classical work extraction and quantum work extraction. Indeed, the model of quantum work extraction is more complicated than that of classical work extraction. This difficulty is mainly caused by the effect of coherence. Hence, Refs. [67,68] proposed how the classical model is close to the quantum model. Although this problem is not directly related to the main issue of this paper, it is nevertheless important, Appendix D gives the answer to this question in the nonasymptotic setting.

APPENDIX B: APPROXIMATION TO THE INTERNAL UNITARY

1. Approximation and coherence

In this section, as another measure of coherence, we focus on the entanglement fidelity

$$F_e(\Lambda,U_I,\rho_I)^2 := \langle\Phi|U_I^\dagger\Lambda(|\Phi\rangle\langle\Phi|)U_I|\Phi\rangle. \tag{B1}$$

When the initial state $|\psi_a\rangle$ is generated with the probability $P_A(a)$, namely, when $\rho_I=\sum_a P_A(a)|\psi_{I,a}\rangle\langle\psi_{I,a}|$ holds, the entanglement fidelity $F_e(\Lambda,U_I,\rho_I)$ characterizes any average fidelity as

$$F_e(\Lambda,U_I,\rho_I)^2 \leqslant \sum_a P_A(a)\langle\psi_a|U_I^\dagger\Lambda(|\psi_a\rangle\langle\psi_a|)U_I|\psi_a\rangle. \tag{B2}$$

Since this value is zero in the ideal case, this value can be regarded as the amount of disturbance by the time evolution Λ. This quantity satisfies the quantum Fano inequality [see [57] and (8.51) in [69]]

$$\begin{aligned}S_e(\Lambda,\rho_I) &= S_e(\Lambda_{U_I^\dagger}\circ\Lambda,\rho_I)\\ &\leqslant h(F_e(\Lambda,U_I,\rho_I)^2)+[1-F_e(\Lambda,U_I,\rho_I)^2]\\ &\quad\times \log\left(d_I^2-1\right),\end{aligned} \tag{B3}$$

where $\Lambda_{U_I^\dagger}(\rho):=U_I^\dagger\rho U_I$. Since this value is also zero in the ideal case, we consider that this value is another measure of the disturbance by the time evolution Λ.

2. Correlation with external system

Next we discuss the correlation with the external system by using the fidelity. We notice another expression of $I_{\rho''_{ZE}}(Z;E)$ as

$$I_{\rho''_{ZE}}(Z;E) = \min_{\sigma_E} D(\rho''_{ZE}\|\rho''_Z\otimes\sigma_E). \tag{B4}$$

Following this expression, we consider the fidelity-type mutual information as

$$I_{F,\rho''_{ZE}}(Z;E) := -\log\max_{\sigma_E} F(\rho''_{ZE},\rho''_Z\otimes\sigma_E). \tag{B5}$$

We can show the following theorem.

Theorem 5. The relations

$$\begin{aligned}I_{F,\rho''_{ZE}}(Z;E) &= -\log\sum_{z,z} P_Z(z)P_Z(z')F(\rho''_{E|Z=z},\rho''_{E|Z=z'})\\ &\leqslant S_2(P_Z)\end{aligned} \tag{B6}$$

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

Theorem 5 follows from a more general argument, Lemma 21 in Appendix E.

Since the equality in (B6) holds in the ideal case, we introduce another measure of the imperfectness of the correlation for the decrease of the energy as

$$\Delta I_{F,\rho''_{ZE}}(Z;E) := S_2(P_Z) - I_{F,\rho''_{ZE}}(Z;E). \tag{B7}$$

Lemma 13. Let $\mathcal{F}=(\mathcal{H}_E,\hat{H}_E,U,\rho_E)$ be an FQ work extraction. Assume that ρ_I is commutative with $\hat{H}_I$. When the CP work extraction $CP(\mathcal{F})$ is a level-4 CP work extraction, the states $\{\rho''_{E|Z=z}\}_z$ are distinguishable.

Proof. Let w_0 be the eigenvalue of the Hamiltonian associated with the state ρ_E. Then

$$\mathrm{Tr}P_{w_0+z'}\rho''_{E|Z=z} = \delta_{z,z'}. \tag{B8}$$

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

Remark 1. We should note the relation between the fidelity-type mutual information $I_{F,\rho''_{ZE}}(Z;E)$ and an existing mutual information measure. A different type of quantum Rényi relative entropy $\tilde{D}_\alpha(\tau\|\sigma)$ was introduced [70,71]. When the order is $\frac{1}{2}$, it is written as

$$\tilde{D}_{\frac{1}{2}}(\tau\|\sigma) = -2\log F(\tau,\sigma). \tag{B9}$$

Using this relation, Refs. [70,72,73] introduced the quantity $\tilde{I}_{\alpha,\rho}(Z;E)$ with general order α by

$$\tilde{I}_{\alpha,\rho}(Z;E) := \min_{\sigma_E}\tilde{D}_\alpha(\rho\|\rho_Z\otimes\sigma_E), \tag{B10}$$

whose operational meaning was clarified by [74]. So our fidelity-type mutual information $I_{F,\rho}(Z;E)$ is written as

$$2I_{F,\rho}(Z;E) = \tilde{I}_{\frac{1}{2},\rho}(Z;E). \tag{B11}$$

3. Trade-off with imperfection of correlation

We derive the fidelity version of the trade-off relation with imperfectness of correlation. To give this kind of trade-off relation, we prepare the isometry V_{IRZ} from $\mathcal{H}_I\otimes\mathcal{H}_R$ to $\mathcal{H}_I\otimes\mathcal{H}_R\otimes\mathcal{H}_Z$:

$$V_{IRZ} := \sum_z |z\rangle\otimes F_z. \tag{B12}$$

Then we define the distribution

$$\tilde{P}_Z(z) := \langle\Phi|U_I^\dagger F_z U_I|\Phi\rangle \tag{B13}$$

and the pure states $|\psi''_{IRE|Z=z}\rangle$ and $|\tilde{\psi}''_{IR|Z=z}\rangle$ by

$$V_{IRZ}U_I|\Phi\rangle = \sum_z \sqrt{\tilde{P}_Z(z)}|\tilde{\psi}_{IR|Z=z},z\rangle, \tag{B14}$$

$$V_{IRZ}U|\Phi,\psi_E\rangle = \sum_z \sqrt{P_Z(z)}|\psi''_{IRE|Z=z},z\rangle. \tag{B15}$$

Theorem 6. The quality of the approximation $F_e(\Lambda,U_I,\rho_I)$ and the amount of imperfectness of the correlation $\Delta I_{F,\rho''_{ZE}}(Z;E)$ satisfy the following trade-off relation:

$$-\log F_e(\Lambda,U_I,\rho_I) + \Delta I_{F,\rho''_{ZE}}(Z;E) \geqslant S_2(P_Z), \tag{B16}$$

i.e.,

$$-\log F_e(\Lambda,U_I,\rho_I) \geqslant I_{F,\rho''_{ZE}}(Z;E). \tag{B17}$$

The equality holds if and only if $\tilde{P}_Z = P_Z$ and there exist pure states $|\psi''_{E|Z=z}\rangle$ such that $|\psi''_{IRE|Z=z}\rangle = |\tilde{\psi}''_{IR|Z=z},\psi''_{E|Z=z}\rangle$ and $\langle\psi''_{E|Z=z'}|\psi''_{E|Z=z}\rangle \geqslant 0$:

$$\begin{aligned}-\log F_e(\Lambda,U_I,\rho_I) &= I_{F,\rho''_{ZE}}(Z;E)\\ &= -\log\sum_{z,z'} P_Z(z)P_Z(z')\langle\psi_{E|Z=z}|\psi_{E|Z=z'}\rangle.\end{aligned} \tag{B18}$$

Proof. Since $F(U_I|\Phi\rangle\langle\Phi|U_I^\dagger,\rho''_{IR}) = F(V_{ZIR}U_I|\Phi\rangle\langle\Phi|U_I^\dagger V_{ZIR}^\dagger, V_{ZIR}\rho''_{IR}V_{ZIR}^\dagger)$, the inequality (B16) is equivalent to

$$\begin{aligned}&F(V_{ZIR}U_I|\Phi\rangle\langle\Phi|U_I^\dagger V_{ZIR}^\dagger, V_{ZIR}\rho''_{IR}V_{ZIR}^\dagger)\\ &\leqslant \max_{\sigma_E} F(\rho''_{ZE},\rho''_Z\otimes\sigma_E).\end{aligned} \tag{B19}$$

So the desired argument follows from Lemma 22 in Appendix E. ■

Here it is better to explain the difference between Theorems 6 and 3. Theorem 3 gives the relation between the decoherence $S_e(\Lambda,\rho_I)$ and the imperfectness of the correlation $\Delta I_{\rho''_{ZE}}(Z;E)$; it does not require any relation with the internal unitary U_I. To derive a relation with the approximation, we employ the quantum Fano inequality (B3). However, Theorem 6 directly gives the relation between the approximation $-\log F_e(\Lambda,U_I,\rho_I)$ and the imperfectness of the correlation $\Delta I_{F,\rho''_{ZE}}(Z;E)$. Hence, it requires the condition (B13).

4. Shift-invariant model

Next we consider how to realize the case when the amount of decoherence $-\log F_e(\Lambda,U_I,\rho_I)$ is close to zero and show Theorem 4. For simplicity, we consider this problem under the shift-invariant model without an additional external system. In the shift-invariant model, once we fix the energy-conservative unitary operator $F[U_I]$ on $\mathcal{H}_I\otimes\mathcal{H}_E$ according to (28), the assumption of Theorem 6 holds and the distribution P_Z depends only on the initial state ρ_I on the system I. That is, P_Z does not depend on the initial state $|\psi_E\rangle$ on the external system E. In this case, we have

$$|\psi_{E|Z=h_E j}\rangle = V^j|\psi_E\rangle. \tag{B20}$$

In particular, when $|\psi_E\rangle = \sum_j \sqrt{P_J(j)}|j\rangle$, the equality condition holds in the inequality (B16). Theorem 6 implies that

$$\begin{aligned}&-\log F_e(\Lambda,U_I,\rho_I)\\ &= I_{F,\rho''_{ZE}}(Z;E)\\ &= -\log\sum_{z,z'} P_Z(z)P_Z(z')\sum_j \sqrt{P_J(j)}\sqrt{P_J(j+z-z')}.\end{aligned} \tag{B21}$$

For example, when

$$P_J(j) = \begin{cases}\frac{1}{2m+1} & \text{if } |j|\leqslant m\\ 0 & \text{otherwise},\end{cases} \tag{B22}$$

$$P_Z(h_E j) = 0 \quad \text{if } |j|\geqslant l, \tag{B23}$$

we have

$$\begin{aligned}-\log F_e(\Lambda,U_I,\rho_I) &= I_{F,\rho''_{ZE}}(Z;E)\\ &\leqslant -\log\left(1-\frac{l}{2m+1}\right) \leqslant \frac{l}{2m+1}.\end{aligned} \tag{B24}$$

Hence, applying (B3), we have

$$\begin{aligned}S_e(\Lambda,\rho_I) &\leqslant h\left(\left(1-\frac{l}{2m+1}\right)^2\right)\\ &\quad+\left[1-\left(1-\frac{l}{2m+1}\right)^2\right]\log\left(d_I^2-1\right)\\ &= h\left(2\frac{l}{2m+1}-\left(\frac{l}{2m+1}\right)^2\right)\\ &\quad+\left[2\frac{l}{2m+1}-\left(\frac{l}{2m+1}\right)^2\right]\log\left(d_I^2-1\right).\end{aligned} \tag{B25}$$

Hence, we obtain Theorem 4.

5. Trade-off under CP work extraction

In Appendix B3 we discussed the trade-off relation between the imperfectness of the correlation and the quality of the approximation under an FQ work extraction. In this section we discuss the trade-off relation under a CP work extraction $\mathcal{G} := \{\mathcal{E}_j,w_j\}_j$ on the internal system $\mathcal{H}_I$ with the Hamiltonian $\hat{H}_I$. To discuss the trade-off relation, in the internal system $\mathcal{H}_I$, we consider the internal unitary U_I to be approximated and the initial mixture state ρ_I is assumed to be commutative with $\hat{H}_I$. To qualify the approximation, we employ the measure $F_e(\sum_j \mathcal{E}_j,U_I,\rho_I)$. To evaluate the imperfectness of correlation, we consider the purification $|\Phi\rangle$ of ρ_I and introduce the joint distribution P_{ZW} as

$$P_{ZW}(z,w) := \sum_{j:w_j=w} \mathrm{Tr}_{RI}\mathcal{E}_j(|\Phi\rangle\langle\Phi|)E_z, \tag{B26}$$

where the projection E_z is defined in the same way as in Sec. V B. Then we employ the measure as $\Delta I_{F,P_{ZW}}(Z;W) = S_2(P_Z) - I_{F,P_{ZW}}(Z;W)$.

As a corollary of Theorem 6, we have the following.

Corollary 3. Given a CP work extraction $\{\mathcal{E}_j,w_j\}_j$, the quality of the approximation $F_e(\sum_j \mathcal{E}_j,U_I,\rho_I)$ and the amount of imperfectness of the correlation $\Delta I_{F,P_{ZE}}(Z;E)$ satisfy the following trade-off relation:

$$-\log F_e\left(\sum_j \mathcal{E}_j,U_I,\rho_I\right)+\Delta I_{F,P_{ZE}}(Z;E)\ \geqslant S_2(P_Z). \tag{B27}$$

Proof. Notice that Theorem 6 does not assume any energy-conservation law. Then we take a Stinespring representation $(\mathcal{H}_E,U,\rho_E)$ with a pure state ρ_E of $\{\mathcal{E}_j,w_j\}_{j\in\mathcal{J}}$ as

$$\mathcal{E}_j(\rho_I)=\mathrm{Tr}_E U_{IE}(\rho_I\otimes\rho_E)U_{IE}^{\dagger}(\hat{1}_I\otimes E_j), \tag{B28}$$

where $\{E_j\}$ is a projection-valued measure on $\mathcal{H}_E$. Notice that $(\mathcal{H}_E,U,\rho_E)$ is an FQ work extraction. Here we do not care whether the FQ work extraction satisfies any energy-conservation law. Then we apply Theorem 6. Since information processing inequality for the fidelity yields that $I_{F,\rho''_{ZE}}(Z;E)\geqslant I_{F,P_{ZE}}(Z;E)$, the relation (B16) derives (B27). ■

Further, we have the following corollary.

Corollary 4. Assume that ρ_I is commutative with $\hat{H}_I$. For a level-4 CP work extraction $\{\mathcal{E}_j,w_j\}_j$, $\Delta I_{P_{ZE}}(Z;E)=\Delta I_{F,P_{ZE}}(Z;E)=0$. So we have

$$-\log F_e\left(\sum_j \mathcal{E}_j,U_I,\rho_I\right)\geqslant S_2(P_Z). \tag{B29}$$

This corollary implies that the dynamics of a level-4 CP work extraction is far from any internal unitary.

APPENDIX C: SHIFT-INVARIANT MODEL WITH A NONLATTICE HAMILTONIAN

Now we show that our discussion for the shift-invariant model in Sec. IV can be extended to the case with nonlattice Hamiltonians $\hat{H}_I$. In this case, we cannot employ the space $L^2(\mathbb{Z})$ for the nondegenerate external system $E1$. One idea is to replace the space $L^2(\mathbb{Z})$ by the space $L^2(\mathbb{R})$. However, in this method, to satisfy the condition (7) with the measurement of the Hamiltonian $\hat{H}_{E1}$, we need to prepare the state whose wave function is a δ function. To avoid such a mathematical difficulty, we employ another construction of the nondegenerate external system $E1$.

Let $\{h_i\}$ be the set of eigenvalues of $\hat{H}_I$. We choose the set $\{h_{E,l}\}_{l=1}^L$ satisfying the following. (i) When rational numbers $t_1,\dots,t_L$ satisfy $\sum_{l=1}^L t_l h_{E,l}=0$, the equality $t_l=0$ holds for all l. (ii) Here $\{h_i-h_j\}_{i,j}\subset\{\sum_{l=1}^L n_l h_{E,l}\}_{n_l\in\mathbb{Z}}$. Then we choose $\mathcal{H}_{E1}$ to be $L^2(\mathbb{Z})^{\otimes L}$ and the Hamiltonian $\hat{H}_{E1}$ to be $\sum_{j_1,\dots,j_L} h_{E,1}j_1+\cdots+h_{E,L}j_L|j_1,\dots,j_L\rangle\langle j_1,\dots,j_L|$.

As in the lattice case, the external system $E1$ does not have a ground state. Because $E1$ in the present case is composed of L ladder systems, we can reconstruct the property of $E1$ in L pairs of harmonic oscillators (see Sec. IV of the Supplemental Material in [45]). Then a shift-invariant unitary is defined as follows. We define L displacement operators $V_{E1,l}:=\sum_j |j+1\rangle_{E\,E}\langle j|$ on the lth space $L^2(\mathbb{Z})$.

Definition 13 (shift-invariant unitary). A unitary U on $\mathcal{H}_I\otimes\mathcal{H}_{E1}$ is called shift invariant when

$$UV_{E1,l}=V_{E1,l}U \tag{C1}$$

for $l=1,\dots,L$.

Then the definition of $F[U_I]$ is changed to

$$F[U_I]:=\sum_{j_1,\dots,j_L}\left(\otimes_{l=1}^L V_{E1,l}^{j_l}\right)WU_IW^{\dagger}\left(\otimes_{l=1}^L V_{E1,l}^{j_l}\right)^{\dagger}. \tag{C2}$$

Under this replacement, we have Lemma 6. Other definitions and lemmas in Sec. IV work with this replacement.

APPENDIX D: CLASSICAL WORK EXTRACTION

1. Formulation

Here we consider again the relation with work extraction from a classical system. Since the original Jarzynski formulation [12] considers only the deterministic time evolution, we need to give a formulation of probabilistic time evolution in the classical system as an extension of Jarzynski's formulation. That is, our formulation can be reduced into the probabilistic work extraction from the classical systems, which is defined as follows.

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

This model includes the previous fully classical scenario [12–18,22], in which we extract work from classical systems. For example, the setup of the Jarzynski equality [12] is a special case that $T(x|x')$ is *invertible and deterministic*, i.e., $T(x|x')$ is given as $\delta_{x,f(x')}$ with an invertible function f. We call such a transition matrix invertible and deterministic. In this case, the transition matrix T is simply written as f_*. That is, for a distribution P, we have

$$f_*(P)(x)=P(f^{-1}(x)). \tag{D1}$$

Notice that the relation

$$(g\circ f)_*(P)=g_*(f_*(P)) \tag{D2}$$

holds. When the transition matrix T is *bistochastic*, i.e., $\sum_x T(x|x')=1$, there exist a set of invertible functions f_l and a distribution $P_L(l)$ such that $T=\sum_l P_L(l)f_{l*}$, i.e.,

$$T(x|x')=\sum_l P_L(l)\delta_{x,f_l(x')}. \tag{D3}$$

This relation means that a bistochastic transition matrix T can be realized by a randomized combination of invertible and deterministic dynamics.

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

$$w_{x,x'}=h_X(x)-h_X(x') \tag{D4}$$

when the initial and final states are x and x'. More generally, the initial state is given as a probability distribution P_X on $\mathcal{X}$.

In this case, the amount of the extracted work is w with the probability

$$\sum_{x',x:w=h_X(x)-h_X(x')} P(x)T(x'|x). \tag{D5}$$

For the entropy of the amount of extracted work, we can show the following lemma in the same way as Lemma 2.

Lemma 14. We denote the random variable describing the amount of extracted work by W. The entropy of W is evaluated as

$$S[W] \leqslant 2\log N, \tag{D6}$$

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

Indeed, our CP work extraction determines the amount of extracted work probabilistically dependently on the initial state on the internal system. So our CP work extraction can be regarded as a natural quantum extension of a probabilistic classical work extraction.

2. Relation to CP work extraction

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

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

$$T_{\{\mathcal{E}_j,w_j\}}(y|x) := \sum_j \langle y|\mathcal{E}_j(\Pi_x)|y\rangle \tag{D7}$$

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

Hence, when the support of the initial state ρ_I of an FQ work extraction $\mathcal{F} = (\mathcal{H}_E,\hat{H}_E,U,\rho_E)$ belongs to an eigenspace of the Hamiltonian $\hat{H}_E$, its classical description is given as $\mathcal{T}(CP(\mathcal{F}))$. The above classical description gives the behavior of a given level-4 CP work extraction $\{\mathcal{E}_j,w_j\}$. When the initial state of the internal system I is the eigenstate $|x\rangle$, due to the condition (2), the amount of the extracted work is w with the probability

$$\sum_{j:w=w_j}\sum_{y:w_j=h_x-h_y} \langle y|\mathcal{E}_j(\Pi_x)|y\rangle = \sum_{y:w=h_x-h_y} T_{\{\mathcal{E}_j,w_j\}}(y|x). \tag{D8}$$

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

Theorem 15. Assume that $\mathcal{P}_{\hat{H}_I}(\rho_I)$ is written as $\sum_x P_X(x)\Pi_x$. [For the definition of $\mathcal{P}_{\hat{H}_I}(\rho_I)$, see (8)]. When we apply a level-4 CP work extraction $\{\mathcal{E}_j,w_j\}$ to the system I with the initial state ρ_I, the amount of the extracted work is w with the probability

$$\sum_{x,y:w=h_x-h_y} T_{\{\mathcal{E}_j,w_j\}}(y|x)P_X(x). \tag{D9}$$

Proof. Due to Lemma 1, the probability of the amount of the extracted work w is

$$\begin{aligned}\sum_{j:w_j=w}\mathrm{Tr}\mathcal{E}_j(\rho) &= \sum_j \mathrm{Tr}\mathcal{P}_{\hat{H}_I}(\mathcal{E}_j(\rho))\delta_{w,w_j}\\ &= \sum_j \mathrm{Tr}\mathcal{E}_j(\mathcal{P}_{\hat{H}_I}(\rho))\delta_{w,w_j}\\ &= \sum_j\sum_{x,y} P_X(x)\langle y|\mathcal{E}_j(\Pi_x)|y\rangle\delta_{w,w_j}\\ &\overset{(a)}{=} \sum_j\sum_{x,y} P_X(x)\langle y|\mathcal{E}_j(\Pi_x)|y\rangle\delta_{w,w_j}\delta_{w_j,h_x-h_y}\\ &= \sum_j\sum_{x,y} P_X(x)\langle y|\mathcal{E}_j(\Pi_x)|y\rangle\delta_{w,h_x-h_y}\delta_{w_j,h_x-h_y}\\ &\overset{(b)}{=} \sum_j\sum_{x,y} P_X(x)\langle y|\mathcal{E}_j(\Pi_x)|y\rangle\delta_{w,h_x-h_y}\\ &\overset{(c)}{=} \sum_{x,y:w_j=h_x-h_y} T_{\{\mathcal{E}_j,w_j\}}(y|x)P_X(x),\end{aligned} \tag{D10}$$

where (a) and (b) follow from (2) and (c) follows from (D7). ■

Due to this theorem, in order to discuss the amount of extracted work in the level-4 CP work extraction, it is sufficient to handle the classical description. Theorem 14 is written as a general form and contains the case when the initial state ρ_I is commutative with the Hamiltonian. In this commutative case, the amount of extracted work can be simulated by the classical model.

Lemma 16. Given a level-4 CP work extraction $\{\mathcal{E}_j,w_j\}$, when the CP work extraction $\{\mathcal{E}_j,w_j\}$ is unital, the transition matrix $T_{\{\mathcal{E}_j,w_j\}}$ is bistochastic.

Proof. Since

$$\sum_j \langle y|\mathcal{E}_j\left(\frac{\hat{1}}{|\mathcal{X}|}\right)|y\rangle = T_{\{\mathcal{E}_j,w_j\}}(y|x)\frac{1}{|\mathcal{X}|}, \tag{D11}$$

when the CP work extraction $\{\mathcal{E}_j,w_j\}$ is unital, the transition matrix $T_{\{\mathcal{E}_j,w_j\}}$ is bistochastic. ■

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

Lemma 17 will be shown after Lemma 18. Since the set of standard FQ work extractions is considered as the set of preferable work extraction, it is sufficient to optimize the performance under the set of classical work extractions with a bistochastic transition matrix. That is, both models yield the same distribution of the amount of extracted work. So our model can be applied in the discussion for the tail probability and the variance for the amount of work extraction as well as the expectation.

As a subclass of bistochastic matrices, we consider the set of unistochastic matrices. A bistochastic matrix T is called unistochastic when there exists a unitary matrix U such that $T(x|x') = |U_{x,x'}|^2$. According to the discussion in Sec. IV and Appendix C, we can consider an FQ work extraction $\mathcal{F} = (\mathcal{H}_{E1},\hat{H}_E,F[U_I],\rho_E)$, where ρ_E is a pure eigenstate of $\hat{H}_E$. As mentioned at the end of Sec. IV, since the corresponding CP work extraction CP($\mathcal{F}$) depends only on the internal unitary U_I, the CP work extraction is denoted by $\hat{\mathrm{CP}}(U_I)$. Then we have the following lemma.

Lemma 18. Given a classical work extraction $(\mathcal{X},h_X,T)$, when the transition matrix T is a unistochastic matrix satisfying $T(x|x') = |U_{I;x,x'}|^2$ with an internal unitary U_I then

$$(\mathcal{X},h_X,T) = \mathcal{T}(\hat{CP}(U_I)). \tag{D12}$$

In the corresponding FQ work extraction $\mathcal{F} = (\mathcal{H}_{E1},\hat{H}_E,F[U_I],\rho_E)$, the entropy of the final state of external system is given as

$$S[W] \geqslant S(\mathrm{Tr}_I F[U_I](\rho_I \otimes \rho_E)F[U_I]^\dagger) \tag{D13}$$

for any pure eigenstate ρ_E of $\hat{H}_E$.

Proof. The relation (D12) can be shown from the definition of $\hat{\mathrm{CP}}(U_I)$. The relation (D13) can be shown in the same way as (6). ∎

Proof of Lemma 17. Given a bistochastic matrix T, there exist a probability distribution $P_A(a)$ and a unitary matrix $U_{I;a}$ such that

$$T(y|x) = \sum_u P_A(a)|U_{I;a;x,y}|^2. \tag{D14}$$

Then we choose the fully degenerate system $\mathcal{H}_{E2}$ spanned by $\{|a\rangle_{E2}\}$ and the initial state $\rho_{E2} := \sum_a P_A(a)|a\rangle_{E2\,E2}\langle a|$. We define the unitary $U := \sum_a F[U_{I;a}] \otimes |a\rangle_{E2\,E2}\langle a|$. So we have $(\mathcal{X},h_X,T) = \mathcal{T}(\mathcal{H}_E,\hat{H}_E,U,\rho_{E1} \otimes \rho_{E2})$ for any pure state ρ_{E1} on $\mathcal{H}_{E1}$. ∎

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

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

$$U_f : |x\rangle \mapsto |f(x)\rangle \tag{D15}$$

satisfies $(\mathcal{X},h_X,T) = \mathcal{T}(\mathcal{H}_{E1},\hat{H}_E,F[U_f],\rho_E)$.

Therefore, any invertible and deterministic transition matrix T can be simulated by a shift-invariant FQ work extraction only with the nondegenerate external system. So the reduction to classical work extraction will be helpful in analyzing the heat engine. That is, in several settings, the analysis of the heat engine can be essentially reduced to the analysis of classical work extraction.

APPENDIX E: RELATIONS AMONG FIDELITIES ON THE TRIPARTITE SYSTEM

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

Lemma 20. We state the following:

$$F(|\Psi\rangle\langle\Psi|,\rho_{AB}) = \sum_{a,a'} \sqrt{\tilde{P}_A(a)P_A(a)}\sqrt{\tilde{P}_A(a')P_A(a')}\langle\phi_{C|a'}|\phi_{C|a}\rangle. \tag{E1}$$

Proof. We show that

$$\begin{aligned}
&F(|\Psi\rangle\langle\Psi|,\rho_{AB})\\
&= \max_{|\psi_C\rangle} F(|\Psi\rangle\langle\Psi||\psi_C\rangle\langle\psi_C|,|\Phi\rangle\langle\Phi|)^2\\
&= \max_{|\psi_C\rangle} \left|\sum_z \sqrt{\tilde{P}_A(a)P_A(a)}\langle\psi_{B|a},\psi_C|\phi_{BC|a}\rangle\right|\\
&= \max_{|\psi_C\rangle} \left|\sum_z \sqrt{\tilde{P}_A(a)P_A(a)}|\phi_{C|a}\rangle\right|\\
&= \sum_{a,a'} \sqrt{\tilde{P}_A(a)P_A(a)}\sqrt{\tilde{P}_A(a')P_A(a')}\langle\phi_{C|a'}|\phi_{C|a}\rangle.
\end{aligned} \tag{E2}$$

∎

Lemma 21. When ρ_{AC} is written as $\sum_a P_A(a)|a\rangle\langle a| \otimes \rho_{C|a}$, we have

$$\max_{\sigma_C} F(\rho_{AC},\rho_A \otimes \sigma_C) = \sum_{a,a'} P_A(a)P_A(a')F(\rho_{C|a},\rho_{C|a'}). \tag{E3}$$

Proof. We first show the case when the state $\rho_{C|a}$ is a pure state $|\phi_{C|a}\rangle$. We choose the purification $|\Phi(\{e^{i\theta_a}\})\rangle := \sum_a e^{i\theta_a}\sqrt{\tilde{P}_A(a)}|a,a,\phi_{C|a}\rangle$ of ρ_{AC} on $\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C$ and the purification $|\Psi(\{e^{i\theta'_a}\})\rangle := \sum_a e^{i\theta'_a}\sqrt{\tilde{P}_A(a)}|a,a\rangle$ of ρ_A on $\mathcal{H}_A \otimes \mathcal{H}_B$. Applying Lemma 20, we have

$$\begin{aligned}
&\max_{\sigma_C} F(\rho_{AC},\rho_A \otimes \sigma_C)\\
&= \max_{\sigma_C} \max_{\{e^{i\theta_a}\},\{e^{i\theta'_a}\}} F(\Pi_{\Psi(\{e^{i\theta'_a}\})} \otimes \sigma_C,\Pi_{\Phi(\{e^{i\theta_a}\})})\\
&= \max_{\{e^{i\theta_a}\},\{e^{i\theta'_a}\}} \max_{\sigma_C} F(\Pi_{\Psi(\{e^{i\theta'_a}\})} \otimes \sigma_C,\Pi_{\Phi(\{e^{i\theta_a}\})})\\
&= \max_{\{e^{i\theta_a}\},\{e^{i\theta'_a}\}} F(\Pi_{\Psi(\{e^{i\theta'_a}\})},\mathrm{Tr}_C\Pi_{\Phi(\{e^{i\theta_a}\})})\\
&= \max_{\{e^{i\theta_a}\},\{e^{i\theta'_a}\}} \sum_{a,a'} e^{i(\theta_a-\theta'_a)-i(\theta'_a-\theta_a)}P_A(a)P_A(a')\langle\phi_{C|a'}|\phi_{C|a}\rangle\\
&= \sum_{a,a'} e^{i(\theta_a-\theta'_a)-i(\theta'_a-\theta_a)}P_A(a)P_A(a')|\langle\phi_{C|a'}|\phi_{C|a}\rangle|,
\end{aligned} \tag{E4}$$

where we use the abbreviations

$$\Pi_{\Psi(\{e^{i\theta'_a}\})} := |\Psi(\{e^{i\theta'_a}\})\rangle\langle\Psi(\{e^{i\theta'_a}\})|, \tag{E5}$$

$$\Pi_{\Phi(\{e^{i\theta_a}\})} := |\Phi(\{e^{i\theta_a}\})\rangle\langle\Phi(\{e^{i\theta_a}\})|. \tag{E6}$$

The equality (E4) implies (E3).

Now we consider the general case. We fix a purification $|\phi_{CD|a}\rangle$ of $\rho_{C|a}$ on $\mathcal{H}_C \otimes \mathcal{H}_D$ so that $F(\rho_{C|a},\rho_{C|a'}) = |\langle\phi_{C|a'}|\phi_{C|a}\rangle|$. We choose the purification $|\Phi(\{e^{i\theta_a}\})\rangle := \sum_a e^{i\theta_a}\sqrt{\tilde{P}_A(a)}|a,a,\phi_{CD|a}\rangle$ of ρ_{AC} on $\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C \otimes \mathcal{H}_D$ and the purification $|\Psi(\{e^{i\theta'_a}\})\rangle := \sum_a e^{i\theta'_a}\sqrt{\tilde{P}_A(a)}|a,a\rangle$ of ρ_A on $\mathcal{H}_A \otimes \mathcal{H}_B$. Similarly, we have

$$\begin{aligned}
&\max_{\sigma_C} F(\rho_{AC},\rho_A \otimes \sigma_C)\\
&= \max_{\sigma_{CD}} \max_{\{e^{i\theta_a}\},\{e^{i\theta'_a}\}} F(\Pi_{\Psi(\{e^{i\theta'_a}\})} \otimes \sigma_{CD},\Pi_{\Phi(\{e^{i\theta_a}\})})
\end{aligned}$$

$$= \max_{\{e^{i\theta_a}\},\{e^{i\theta'_a}\}} \max_{\sigma_{CD}} F(\Pi_{\Psi(\{e^{i\theta'_a}\})} \otimes \sigma_{CD}, \Pi_{\Phi(\{e^{i\theta_a}\})})$$
$$= \sum_{a,a'} e^{i(\theta_a-\theta'_a)-i(\theta'_a-\theta_a)} P_A(a)P_A(a')|\langle\phi_{C|a'}|\phi_{C|a}\rangle|$$
$$= \sum_{a,a'} e^{i(\theta_a-\theta'_a)-i(\theta'_a-\theta_a)} P_A(a)P_A(a')F(\rho_{C|a},\rho_{C|a'}), \quad \text{(E7)}$$

which implies (E3). ■

Lemma 22. When $P_A = \tilde{P}_A$,

$$F(|\Phi\rangle\langle\Phi|,\rho_{AB}) \leqslant \max_{\sigma_C} F(\rho_{AC},\rho_A \otimes \sigma_C). \quad \text{(E8)}$$

The equality holds if and only if $\langle\phi_{C|a'}|\phi_{C|a}\rangle \geqslant 0$ and $\langle\phi_{C|a}|\phi_{C|a}\rangle = 1$.

Proof. We use the notation in Lemmas 20 and 21. Then we have

$$\langle\phi_{C|a'}|\phi_{C|a}\rangle + \langle\phi_{C|a}|\phi_{C|a'}\rangle \leqslant 2F(\rho_{C|a},\rho_{C|a'}). \quad \text{(E9)}$$

Combining Lemmas 20 and 21, we have

$$F(|\Phi\rangle\langle\Phi|,\rho_{AB})$$
$$= \sum_{a,a'} \sqrt{\tilde{P}_A(a)P_A(a)}\sqrt{\tilde{P}_A(a')P_A(a')}\langle\phi_{C|a'}|\phi_{C|a}\rangle$$
$$\leqslant \sum_{a,a'} P_A(a)P_A(a')F(\rho_{C|a},\rho_{C|a'})$$
$$= \max_{\sigma_C} F(\rho_{AC},\rho_A \otimes \sigma_C). \quad \text{(E10)}$$

Hence, we obtain (E8). The equality in (E8) holds if and only if that in (E9) holds. So we obtain the desired equivalence. ■

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