

# Quantum thermodynamic cycles and quantum heat engines

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In order to describe quantum heat engines, here we systematically study isothermal and isochoric processes for quantum thermodynamic cycles. Based on these results the quantum versions of both the Carnot heat engine and the Otto heat engine are defined without ambiguities. We also study the properties of quantum Carnot and Otto heat engines in comparison with their classical counterparts. Relations and mappings between these two quantum heat engines are also investigated by considering their respective quantum thermodynamic processes. In addition, we discuss the role of Maxwell's demon in quantum thermodynamic cycles. We find that there is no violation of the second law, even in the existence of such a demon, when the demon is included correctly as part of the working substance of the heat engine.

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## I. INTRODUCTION

Quantum heat engines (QHEs) [1,2] produce work using quantum matter as their working substance. Because of the quantum nature of the working substance, QHEs have unusual and exotic properties. For example, under some conditions, QHE can surpass the maximum limit on the amount of work done by a classical thermodynamic cycle [3,4] and also surpass the efficiency of a classical Carnot engine cycle [5]. QHEs offer good model systems to study the relation between thermodynamics and quantum mechanics. Meanwhile, they can highlight the difference between classical and quantum thermodynamic systems, and help us understand the quantum-classical transition problem of thermodynamic processes [6].

The classical Carnot heat engine is a well-known machine that produces work through thermodynamic cycles. The thermodynamic properties of the four strokes of each cycle are simple and demonstrate the universal physical mechanism of heat engines. Current studies [3–14] on QHE mostly focus on the quantum analogue of classical Carnot engines, i.e., the quantum Carnot engine (QCE). The quantum Otto engine (QOE) is another interesting case of a QHE, which is also attracting considerable attention [3,4,15–18]. However, we find that there is no universal and consistent definition of the QCE and the QOE in the literature (see, e.g., Refs. [5,9,10,19,20]), and thus the properties of QCEs and QOE are not always addressed adequately and clearly.

Any QHE cycle consists of several basic quantum thermodynamic processes, such as quantum adiabatic processes (which have been clarified in many references, e.g., [21]), quantum isothermal processes and quantum isochoric processes. This paper begins by clarifying the concepts of isothermal processes, isochoric processes, and effective temperatures in their quantum mechanical pictures. Then we systematically study the general properties of a quantum analogue of a Carnot engine. The difference between a QCE and its classical counterpart is indicated clearly. We also study

the QOE based on its basic quantum thermodynamic process and analyze the relation between these two types of QHEs. Here we assume that the processes of our thermodynamic cycles are infinitely slow, i.e., the time interval of each process is assumed to be very long. Accordingly, the output power is very small. This is also the requirement of quasi-static processes. Assuming fast cycles would increase the output powers, but at the expense of reduced engine efficiency. Also, some experimentally realizable physical systems, which can be used to implement our QCE and QOE, are discussed. Furthermore, based on our generalized QOE model, we demonstrate that there is no violation of the second law, even in the presence of a Maxwell's demon.

Our paper is organized as follows: In Sec. II we give a clear definition of quantum isothermal and isochoric processes based on the quantum identification of work performed and heat exchange. In Sec. III we discuss the QCE cycle and calculate the work done during this cycle and its operation efficiency. In Sec. IV we discuss the QOE cycle and compare it with the classical Otto engine cycle. In Sec. V we compare these two kinds of QHEs and study the relation between them. In Sec. VI we give some examples of these two kinds of QHEs considering experimentally realizable physical systems. In Sec. VII we discuss the QOE and Maxwell's demon. Conclusions and remarks are given in Sec. VIII.

## II. BASIC QUANTUM THERMODYNAMIC PROCESS

### A. Quantum first law of thermodynamics

To define quantum isothermal and quantum isochoric processes, we need to first consider the working substance. An arbitrary quantum system with a finite number of energy levels is used here as the working substance (see Fig. 1). (Of course, this can be generalized to systems with an infinite number of energy levels.) The Hamiltonian of the working substance can be written as

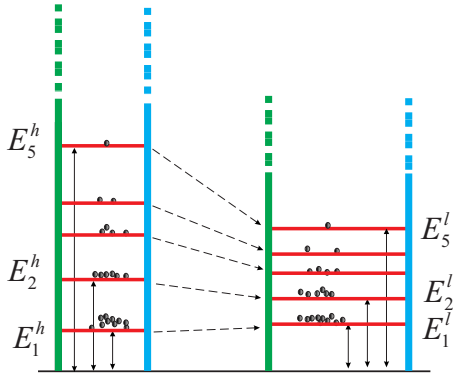


FIG. 1. (Color online) Schematic diagram of multilevel quantum system as the working substance for a QHE.  $E_n^h$  and  $E_n^l$  are the  $n$ th eigenenergy of the working substance in the two isochoric processes.

$$H = \sum_n E_n |n\rangle\langle n|, \quad (1)$$

where  $|n\rangle$  is the  $n$ th eigenstate of the system and  $E_n$  is its corresponding eigenenergy. Without loss of generality, we choose the eigenenergy of the ground state  $|0\rangle$  as a reference point (see Appendix A). Then the Hamiltonian (1) can be rewritten as

$$H = \sum_n (E_n - E_0) |n\rangle\langle n|. \quad (2)$$

Below we will show that it is convenient for our discussion about QHEs to use the Hamiltonian (2). The internal energy  $U$  of the working substance can be expressed as

$$U = \langle H \rangle = \sum_n P_n E_n, \quad (3)$$

for a given occupation distribution with probabilities  $P_n$  in the  $n$ th eigenstate.

To clearly define quantum isothermal and isochoric processes, we need to identify the quantum analogues of the heat exchange  $dQ$  and the work performed  $dW$ . From Eq. (3) we have

$$dU = \sum_n (E_n dP_n + P_n dE_n). \quad (4)$$

In classical thermodynamics, the first law of thermodynamics is expressed as

$$dU = dQ + dW, \quad (5)$$

where  $dQ = TdS$ , and  $dW = \sum_i Y_i dy_i$  [22];  $T$  is the temperature and  $S$  is the entropy;  $y_i$  is the generalized coordinates and  $Y_i$  is the generalized force conjugated to  $y_i$ . Due to the relationship  $S = -k_B \sum_i P_i \ln P_i$  between the entropy  $S$  and the probabilities  $P_i$ , we can make the following identification [3,4,17]

$$dQ = \sum_n E_n dP_n, \quad (6)$$

$$dW = \sum_n P_n dE_n. \quad (7)$$

Equation (7) implies that the work performed corresponds to the change in the eigenenergies  $E_n$ , and this is in accordance with the fact that work can only be performed through a change in the generalized coordinates of the system, which in turn gives rise to a change in the eigenenergies [4,23]. Thus the quantum version of the first law of thermodynamics  $dU = dQ + dW$  just follows from Eq. (4) with the quantum identifications of heat exchange and work performed in Eqs. (6) and (7). Different from  $dQ = TdS$ , which is applicable only to the thermal equilibrium case, below we will see that Eqs. (6) and (7) are applicable to both the thermal equilibrium case [see e.g., Eq. (36)] and the nonequilibrium case [see, e.g., Eq. (21)].

### B. Quantum isothermal process

Let us now consider the quantum versions of some thermodynamic processes. First we study quantum isothermal processes. In quantum isothermal processes, the working substance, such as a particle confined in a potential energy well, is kept in contact with a heat bath at a constant temperature. The particle can perform positive work to the outside, and meanwhile absorb heat from the bath. Both the energy gaps and the occupation probabilities need to change simultaneously, so that the system remains in an equilibrium state with the heat bath at every instant. Specifically, let us consider a two-level system with the excited state  $|e\rangle$ , the ground state  $|g\rangle$ , and a single energy spacing  $\Delta$ . In the quasistatic quantum isothermal process, the ratio  $r = P_e/P_g$  of the two occupation probabilities,  $P_e$  and  $P_g$ , must satisfy the Boltzmann distribution  $r = P_e/P_g = \exp[-\beta\Delta(t)]$  and also the normalization condition  $P_e + P_g = 1$ .  $\Delta(t)$  changes slowly with time  $t$ , and accordingly  $r$  can be written as

$$r \equiv r(t) = \frac{P_e}{P_g} = e^{-\beta\Delta(t)}, \quad (8)$$

where  $\beta = 1/k_B T$ ,  $k_B$  is the Boltzmann constant and  $T$  is the temperature. In a sufficiently slow process, at every instant the system remains in thermodynamic equilibrium with the heat bath.

### C. Effective temperature

We can also define an effective temperature  $T_{\text{eff}}$  for any two-level system according to the ratio  $r(t)$  and the level spacing  $\Delta(t)$ . For a two-level system with energy levels  $E_e$  and  $E_g$ , even in a nonequilibrium state, we can imagine that it is in a virtual equilibrium state with the effective temperature

$$T_{\text{eff}} = \frac{1}{k_B \beta_{\text{eff}}} = \frac{\Delta(t)}{k_B} \left( \ln \frac{P_g}{P_e} \right)^{-1}, \quad (9)$$

as long as the level spacing  $\Delta(t)$  and the energy level distributions  $P_g$  and  $P_e$  are known. Of course, Eq. (9) cannot be directly generalized to the case with more than two levels. For example, for a three-level system with occupation prob-

TABLE I. Quantum vs classical thermodynamic processes. Here we use “INV” to indicate the invariance of a thermodynamic quantity and “VAR” to indicate that it varies or changes.  $U$  is the internal energy of the working substance;  $T, P, E_n, P_n$  are defined in Sec. II. The working substance of the classical thermodynamic processes considered here is the ideal classical gas.

	Isothermal process	Isochoric process	Adiabatic process
Classical	Heat absorbed or released	Heat absorbed or released	No heat exchange
	Work done	No work done	Work done
	INV: $U, T$ VAR: $P, V$	INV: $V$ VAR: $P, T$	VAR: $P, T, V$
Quantum	Heat absorbed or released	Heat absorbed or released	No heat exchange
	Work done	No work done	Work done
	INV: $T$ VAR: $U, E_n, P_n$	INV: $E_n$ VAR: $P_n, T_{\text{eff}}$	INV: $P_n$ VAR: $E_n, T_{\text{eff}}$

abilities  $P_a, P_b$ , and  $P_c$  in three states denoted by  $|a\rangle, |b\rangle$ , and  $|c\rangle$ , if the two-level spacings  $\Delta_{ab}(t)$  and  $\Delta_{bc}(t)$  do not satisfy the relation

$$\frac{1}{\Delta_{ab}(t)} \ln \frac{P_a}{P_b} = \frac{1}{\Delta_{bc}(t)} \ln \frac{P_b}{P_c}, \quad (10)$$

we cannot define a unique effective temperature. The subset  $\{|a\rangle, |b\rangle\}$  can have an effective temperature defined by Eq. (9), while the subset  $\{|b\rangle, |c\rangle\}$  would have a different effective temperature. We will discuss this point in detail in a QCE cycle in Sec. III.

#### D. Quantum isochoric process

A quantum isochoric process has similar properties to that of a classical isochoric process. In a quantum isochoric process, the working substance is placed in contact with a heat bath. No work is done in this process while heat is exchanged between the working substance and the heat bath. This is the same as that in a classical isothermal process. In a quantum isochoric process the occupation probabilities  $P_n$  and thus the entropy  $S$  change, until the working substance finally reaches thermal equilibrium with the heat bath. In a classical isochoric process the pressure  $P$  and the temperature  $T$  change, and the working substance reaches thermal equilibrium with the heat bath only at the end of this process. For example, if the working substance is chosen to be a particle confined in a infinite square well potential, no work is done during a quantum isochoric process when heat is absorbed or released, and the occupation probabilities in every eigenstate satisfy Boltzmann distribution at the end of the isochoric process.

#### E. Quantum adiabatic process

A classical adiabatic thermodynamic process can be formulated in terms of a microscopic quantum adiabatic thermodynamic process. Because quantum adiabatic processes proceed slow enough such that the generic quantum adiabatic condition is satisfied, then the population distributions remain unchanged,  $dP_n=0$ . According to Eq. (6),  $\dot{d}Q=0$ , there is no heat exchange in a quantum adiabatic process, but work can still be nonzero according to Eq. (7). A classical adiabatic process, however, does not necessarily require the

occupation probabilities to be kept invariant. For example, when the process proceeds very fast, and the quantum adiabatic condition is not satisfied, internal excitations will likely occur, but there is no heat exchange between the working substance and the external heat bath. This thermodynamic process is classical adiabatic but not quantum adiabatic. Thus it can be verified that a classical adiabatic process includes, as a subset, a quantum adiabatic process; but the inverse is not valid [17].

The properties of both classical and quantum thermodynamic process are listed in Table I, to facilitate the comparison between these two processes. The table indicates if heat is absorbed or released (first row), if work is done (second row), and which quantity varies (indicated by “VAR”) and which are invariant (indicated by “INV”) in the third row.

### III. QUANTUM CARNOT ENGINE CYCLE

In the preceding section, we defined quantum isothermal processes. Based on this definition, in this section, we study the QCE cycle and its properties. The QCE cycle (see Fig. 2 for an example of a QCE based on a two-level system), just like its classical counterpart, consists of two quantum isothermal processes ( $A \rightarrow B$  and  $C \rightarrow D$ ) and two quantum adiabatic processes ( $B \rightarrow C$  and  $D \rightarrow A$ ). During the isothermal expansion process from  $A$  to  $B$ , the particle confined in the potential well is kept in contact with a heat bath at temperature  $T_h$ , while the energy levels of the system change much slower than the relaxation of the system, so that the particle is always kept in thermal equilibrium with the heat bath. Below, we consider both cases: two-level and multilevel systems.

#### A. Thermodynamic reversibility of the quantum Carnot engine cycle

It is well known that quantum mechanical reversibility is associated with quantum mechanical unitary evolution. Different from quantum mechanical reversibility, thermodynamic reversibility accompanies the heat bath and the effective temperature of the working substance. In this paper we focus on the thermodynamic reversibility.

We emphasize that, in order to ensure that the cycle is thermodynamically *reversible*, two conditions on the quan-

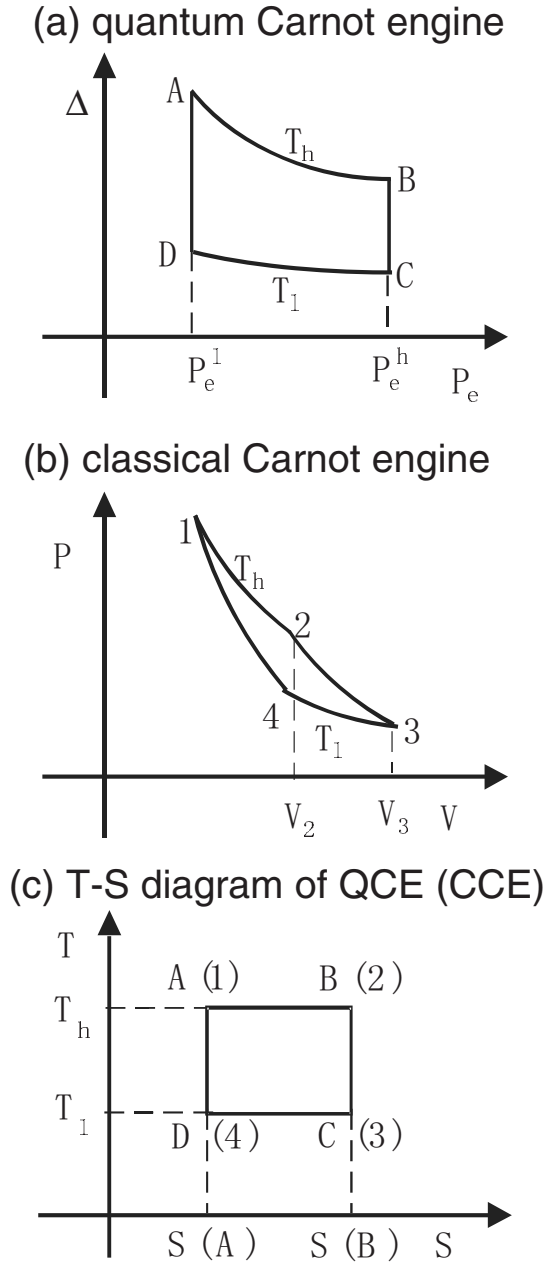


FIG. 2. (a): A schematic diagram of a *quantum* Carnot engine based on a two-level quantum system.  $\Delta$  is the level spacing between the two energy levels.  $P_e$  is the occupation probability in the excited state. The process from A to B (C to D) is the isothermal expansion (compression) process, in which the working substance is put in contact with the high (low) temperature heat bath. The processes from B to C and from D to A are two adiabatic processes. (b): Pressure-volume ( $P$ - $V$ ) diagram for a *classical* Carnot engine with ideal gas as the working substance. The process from 1 to 2 (from 3 to 4) is the classical isothermal expansion (compression) process with temperature  $T_h$  ( $T_l$ ), and the process from 2 to 3 (4 to 1) is the classical adiabatic expansion (compression) process.  $V_2$  and  $V_3$  are the volume of the working substance at 2 and 3, respectively. (c) Temperature-entropy ( $T$ - $S$ ) diagram [27] for both a *quantum* Carnot engine based on a two-level quantum system and a *classical* Carnot engine with ideal gas as the working substance. This  $T$ - $S$  diagram bridges the *quantum* and *classical* Carnot engine.

tum adiabatic process are required: (1) after the quantum adiabatic process ( $B \rightarrow C$ ), we can use an effective temperature  $T_l$  to characterize the working substance, i.e., the working substance still satisfies the Boltzmann distribution after the quantum adiabatic process; and (2) the effective temperature  $T_l$  of the working substance, after the quantum adiabatic process, equals the temperature  $T_l$  of the heat bath of the following quantum isothermal process ( $C \rightarrow D$ ). When either condition is not satisfied, a thermalization process [24,25] of the working substance is inevitable before the quantum isothermal process ( $C \rightarrow D$ ). In the thermalization process, the total entropy increase of the working substance plus the bath is nonzero. Hence, this thermalization process is irreversible.

It can be proved that the above two conditions are equivalent to the following two conditions: (i) all energy gaps were changed by the same ratio in the quantum adiabatic process, i.e.,  $E_n(B) - E_m(B) = \lambda[E_n(C) - E_m(C)]$  and  $E_n(A) - E_m(A) = \lambda[E_n(D) - E_m(D)]$  ( $n=0, 1, 2, \dots$ ); and (ii) the ratio of the change of the energy gaps in the adiabatic process (from B to C or from A to D) must equal the ratio of the two temperatures of the heat baths, i.e.,  $\lambda = T_h/T_l$ .

First, it is easy to see that these two conditions, (i) and (ii), listed above are sufficient for the previous conditions (1) and (2) presented initially. Next, we prove that the two conditions (i) and (ii) are also necessary for the two conditions (1) and (2). Let us assume that the working substance is in equilibrium with a heat bath at temperature  $T_h$  at the instant B before the adiabatic process ( $B \rightarrow C$ ). In this case the quantum state is described by a density operator

$$\rho(B) = \frac{1}{Z} \sum_n \exp[-\beta_h E_n(B)] |n(B)\rangle \langle n(B)|. \quad (11)$$

After the adiabatic process is completed, at instant C in Fig. 2, the eigenenergies of the working substance become  $E_n(C)$ , and the working substance reaches an effective temperature  $T_l$ . The occupation probabilities  $P_n$  of the working substance are kept unchanged during the adiabatic process ( $B \rightarrow C$ ), and they satisfy the Boltzmann distribution. Thus, for any eigenstates  $|n\rangle$  and  $|m\rangle$ , the occupation probabilities  $P_n$  and  $P_m$  satisfy

$$\frac{P_n(B)}{P_m(B)} = \frac{\exp[-\beta_h E_n(B)]}{\exp[-\beta_h E_m(B)]} = \frac{P_n(C)}{P_m(C)} = \frac{\exp[-\beta_l E_n(C)]}{\exp[-\beta_l E_m(C)]}. \quad (12)$$

That is,

$$E_n(C) - E_m(C) = \frac{T_l}{T_h} [E_n(B) - E_m(B)], \quad (13)$$

for any  $m, n$ . Equation (13) is just a combination of conditions (i) and (ii). Thus we have proved that the two conditions (i) and (ii) are sufficient for the previous conditions (1) and (2).

Hence, we have proven that (i) all energy gaps change by the same ratio in the quantum adiabatic process, and (ii) this ratio equals to the ratio of the temperatures of the two heat baths, summarized in Eq. (13), are sufficient and necessary conditions for the QCE to be thermodynamically reversible.



We would like to mention that these two conditions (i) and (ii) (mathematical requirements) can be satisfied in some realistic physical systems. Examples of QCEs based on some concrete physical systems will be discussed in Sec. VI.

### B. Work and efficiency of a quantum Carnot engine cycle

Now we analyze the operation efficiency  $\eta_C$  of the QCE introduced above. For simplicity, instead of applying Eq. (6), we use  $dQ = TdS$  to calculate the heat exchange  $dQ$  in any quantum isothermal (QIT) process. Because the temperature of the heat bath is kept invariant in the quantum isothermal process, the heat absorbed  $Q_{in}^{QIT}$  and released  $Q_{out}^{QIT}$  in the quantum isothermal expansion and compression processes can be calculated as follows:

$$Q_{in}^{QIT} = T_h[S(B) - S(A)] > 0, \quad (14)$$

$$Q_{out}^{QIT} = T_l[S(C) - S(D)] > 0, \quad (15)$$

where  $T_h$  and  $T_l$  are the temperatures of the two different heat baths, and

$$S(i) = -k_B \sum_n \frac{\exp[-\beta_i E_n(i)]}{Z(i)} [-\beta_i E_n(i) - \ln Z(i)], \quad (16)$$

are the entropies of the working substance at different instants  $i=A, B, C, D$  [see Fig. 3(a)]. Here,  $\beta_{A,B} = 1/k_B T_h$ ,  $\beta_{C,D} = 1/k_B T_l$ . In obtaining the above result, we have used the Boltzmann distribution of a thermal equilibrium state, i.e.,  $\rho = (1/Z) \sum_n \exp(-\beta E_n) |n\rangle\langle n|$ , where  $Z = \text{Tr} \exp(-\beta H)$  is the partition function. Of course,  $Q_{in}^{QIT}$  and  $Q_{out}^{QIT}$  can also be obtained through Eq. (6) in a quantum manner [this will become clear later on, see Eqs. (36) and (37)]. These equivalent approaches can describe the microscopic mechanism of a classical Carnot engine cycle.

Now, we would like to calculate the work  $W_C$  done during a QCE cycle and its operation efficiency  $\eta_C$ . From Eqs. (14) and (15) and the first law of thermodynamics we obtain the net work done during a QCE cycle,

$$W_C = Q_{in}^{QIT} - Q_{out}^{QIT} = (T_h - T_l)[S(B) - S(A)], \quad (17)$$

where we have used the relations  $S(B) = S(C)$  and  $S(A) = S(D)$ . This equivalence is due to the fact that the occupation probabilities and thus the entropy remain invariant in any quantum adiabatic process. The efficiency  $\eta_C$  of the QCE is

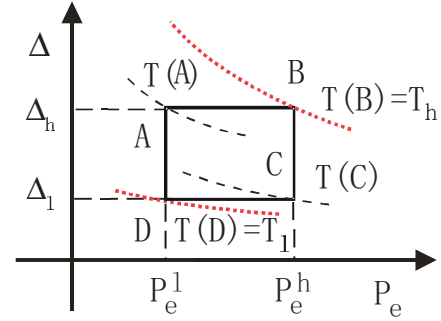
$$\eta_C = \frac{W_C}{Q_{in}^{QIT}} = 1 - \frac{T_l}{T_h}, \quad (18)$$

which is just the efficiency of a classical Carnot engine. From Eq. (13) we see that the ratio of the temperature in the efficiency [Eq. (18)] of the QCE can also be replaced by the ratio of the energy gaps

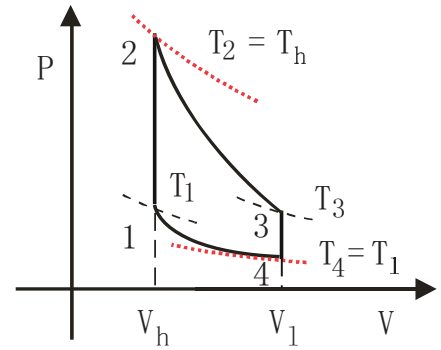
$$\eta_C = 1 - \frac{E_n(C) - E_m(C)}{E_n(B) - E_m(B)}. \quad (19)$$

This expression of the efficiency  $\eta_C$  in terms of the ratio of the energy gaps resembles that of a QOE for a multilevel

### (a) quantum Otto engine



### (b) classical Otto engine



### (c) T-S diagram of QOE (COE)

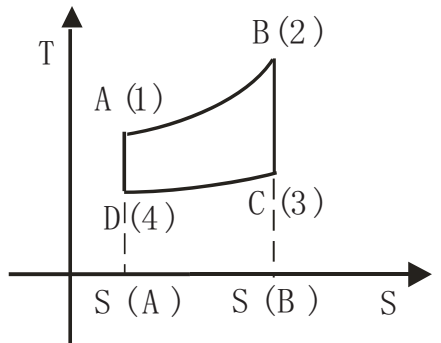


FIG. 3. (Color online) (a) A schematic diagram of a *quantum* Otto engine based on a two-level quantum system. Dotted red and dashed black curves refer to the isothermal processes.  $\Delta_h$  and  $\Delta_l$  are the level spacings of the two-level system during the two isochoric processes ( $A \rightarrow B$  and  $C \rightarrow D$ ).  $P_e^h$  and  $P_e^l$  are the occupation probabilities in the excited state. The processes from  $A$  to  $B$  and from  $C$  to  $D$  are isochoric processes, while the processes from  $B$  to  $C$  and from  $D$  to  $A$  are quantum adiabatic processes.  $T(i)$ , ( $i=A, B, C, D$ ) are the effective temperatures of the working substance at instant  $i$ , and  $T(B) = T_h$ ,  $T(D) = T_l$ . (b) Pressure-volume, ( $P$ - $V$ ), diagram of a *classical* Otto engine.  $V_h$  and  $V_l$  are the volume of the working substance in the two classical isochoric processes. The process from 1 to 2 (3 to 4) is a classical isochoric heating (cooling) process, and the process from 2 to 3 (4 to 1) is the classical adiabatic expansion (compression) process. The temperature of the working substance at 2 and 4 equal to the temperatures of the two heat baths,  $T_h$  and  $T_l$ , respectively. (c) Temperature-entropy ( $T$ - $S$ ) diagram [27] for both a *quantum* Otto engine based on a two-level quantum system and a *classical* Otto engine with ideal gas as the working substance. This  $T$ - $S$  diagram bridges the *quantum* and *classical* Otto engine.

TABLE II. Quantum Carnot engines versus classical Carnot engines. Here ‘‘CIT’’ refers to ‘‘classical isothermal process’’ while ‘‘CA’’ is an abbreviation for a ‘‘classical adiabatic process.’’ ‘‘QIT’’ and ‘‘QA’’ refer to ‘‘Quantum isothermal process’’ and ‘‘quantum adiabatic process,’’ respectively.  $V_2, V_3, E_n(B)$ , and  $E_n(C)$  are defined in Fig. 2;  $\gamma$  is the adiabatic exponent [27].

	Strokes	Requirement on the CA and QA	Efficiency	Positive-work condition
Classical	CIT-CA-CIT-CA	$\frac{T_l}{T_h} = \left(\frac{V_2}{V_3}\right)^{\gamma-1}$	$\eta = 1 - \frac{T_l}{T_h}$	$T_h > T_l$
Quantum	QIT-QA-QIT-QA	$\frac{T_l}{T_h} = \frac{E_n(C) - E_m(C)}{E_n(B) - E_m(B)}$ for $\forall m, n$	$\eta = 1 - \frac{T_l}{T_h}$	$T_h > T_l$

case in Refs. [3,17] [see also Eq. (24) below]. However, in spite of the apparent similarities between these two expressions for the efficiencies, we emphasize that they are quite different. Here,  $E_n(B) - E_m(B)$  and  $E_n(C) - E_m(C)$ , in Eq. (19), are the energy gaps at the beginning ( $B$ ) and at the end ( $C$ ) of the quantum adiabatic expansion process ( $B \rightarrow C$ ). In the expression for the efficiency  $\eta_0$  for a multilevel QOE, however, the energy gaps are those in two quantum isochoric processes [3,17]. Hence, the efficiency in Eq. (19) for a QCE is quite different from that for a QOE, even though they both look similar. Further discussions on this will be given in Sec. IV.

In order to extract positive work from the bath, Eq. (18) imposes a constraint,  $T_h > T_l$ , on the temperatures of the two heat baths. This constraint, known as the positive-work condition (PWC), is the same as that of its classical counterpart. What is more, the schematic temperature-entropy ( $T$ - $S$ ) diagrams for both a QCE cycle and a classical Carnot engine cycle are the same [see Fig. 2(c)]. For the above reasons, we believe it is convincible that our QCE model is a quantum mechanical analogue of a classical Carnot engine. We compare the properties of a QCE and a classical Carnot engine and list them in Table II.

### C. Internal energy

It is well known that an ideal classical Carnot engine cycle consists of two classical isothermal and two classical adiabatic processes. When the working substance is the ideal gas, the internal energy of the working substance remains invariant in the classical isothermal process, because the internal energy of the ideal gas depends on the temperature only. This assumption for classical isothermal processes based on classical ideal gas could be true for a classical Carnot engine using a working substance other than an ideal gas. But in the quantum version, the quantum isothermal and quantum adiabatic processes should be redefined microscopically based on quantum mechanics. In principle, the classical result could change when considering the quantum nature (discrete energy levels) of the working substance.

We now would like to verify whether the internal energy of the working substance remains invariant during the isothermal process. At the four instants  $A, B, C$ , and  $D$  of the QCE cycle (see Fig. 2), the internal energies are, respectively,

$$U(i) = \text{Tr}[\rho(i)H(i)], \quad i = A, B, C, D. \quad (20)$$

In Appendix B we prove that  $U(A) \neq U(B)$  and  $U(C) \neq U(D)$  for some QCE cycles based on several experimen-

tally realizable systems. Hence, in the quantum version of a Carnot engine, we cannot simply assume that the heat absorbed (released) by the working substance is equal to the work done by (on) the working substance in the isothermal process, as we do in classical Carnot engine with the ideal gas as the working substance. This observation is crucial for the following discussion.

Here we would like to indicate that, the quantum isoenergetic process in Refs. [7,8] is not a quantum analogue of the classical isothermal process of a classical Carnot engine, because it requires the temperature of the heat bath to change. Thus the thermodynamic cycle described in Refs. [7,8] is actually not a QCE cycle.

## IV. QUANTUM OTTO ENGINE CYCLE

In practice, the heat engines most widely used in automobiles, the internal combustion engine, operate using Otto-cycle engines [18], which consist of two classical isochoric and two classical adiabatic processes. Similar to the Carnot engine, the quantum analogue of the classical Otto engine is also proposed in Refs. [3,9,10,17,19]. The QOE cycle consists of two quantum isochoric and two quantum adiabatic processes [4,15–17] (see Fig. 3 for a schematic diagram of QOE based on a two-level system).

### A. Work and efficiency

In the quantum isochoric heating process from  $A$  to  $B$  (see Fig. 3), no work is done, but heat is absorbed. The heat  $Q_{\text{in}}^{\text{QIC}}$  absorbed by the working substance is

$$Q_{\text{in}}^{\text{QIC}} = \sum_n \int_A^B E_n dP_n = \sum_n E_n^h [P_n(B) - P_n(A)], \quad (21)$$

where  $E_n^h$  is the  $n$ th eigenenergy of the system in the quantum isochoric heating process from  $A$  to  $B$ . Similarly, we obtain the heat released to the low temperature entropy sink in the quantum isochoric cooling process from  $C$  to  $D$ ,

$$Q_{\text{out}}^{\text{QIC}} = - \sum_n \int_C^D E_n dP_n = \sum_n E_n^l [P_n(C) - P_n(D)], \quad (22)$$

where  $E_n^l$  is the  $n$ th eigenenergy of the system in the quantum isochoric cooling process. We would like to point out that in calculating  $Q_{\text{in}}^{\text{QIC}}$  and  $Q_{\text{out}}^{\text{QIC}}$ , we cannot apply Eqs. (14) and (15), because  $dQ = TdS$  is only applicable to the thermal equilibrium case, while in the quantum isochoric process, the heat bath and the working substance are not always in ther-

mal equilibrium, i.e., this process is not thermodynamically reversible (for a detailed discussion see below).

As mentioned above, in order to construct a QCE, all energy gaps must be changed by the same ratio in a quantum adiabatic process. But for a multilevel QOE, there is no such constraint (see Ref. [17]) because we do not have to ensure the reversibility of the QOE cycle. Nevertheless, to compare the QOE with the QCE, we only consider a special case of QOE where all its energy gaps change by the same ratios as in the quantum adiabatic processes, i.e.,  $E_n^h - E_m^h = \alpha(E_n^l - E_m^l)$ , ( $n=0, 1, 2, \dots$ ). When we choose  $E_0^h = E_0^l = 0$ , i.e., the ground-state eigenenergies as the energy reference point, we have  $E_n^h = \alpha E_n^l$ . Similar to the QCE, the occupation distribution remains invariant in the two quantum adiabatic processes, i.e.,  $P_n(B) = P_n(C)$  and  $P_n(A) = P_n(D)$ , and accordingly the entropy remains invariant in the quantum adiabatic processes  $S(B) = S(C)$  and  $S(A) = S(D)$ .

Based on this fact, and Eqs. (21) and (22), we obtain the net work  $W_O$  done during a QOE cycle

$$W_O = Q_{\text{in}}^{\text{QIC}} - Q_{\text{out}}^{\text{QIC}} = \sum_n (E_n^h - E_n^l) [P_n(B) - P_n(A)], \quad (23)$$

and the operation efficiency  $\eta_O$  of the QOE cycle

$$\eta_O = \frac{W_O}{Q_{\text{in}}^{\text{QIC}}} = 1 - \frac{E_n^l - E_m^l}{E_n^h - E_m^h} = 1 - \frac{1}{\alpha}. \quad (24)$$

Here,  $\alpha > 1$  since  $E_n^h > E_n^l$ . This result, which stands for a special multilevel QOE (all energy gaps change by the same ratio in the quantum adiabatic process), is a generalization of the two-level QOE [3,17]. Let us recall the PWC of the special multilevel QOE [17] mentioned above. From Eq. (23), the PWC for the special multilevel QOE is

$$T_h > \alpha T_l. \quad (25)$$

This is obviously different from that of a QCE, where the PWC is simply  $T_h > T_l$ .

Note that the first QHE model, initially proposed in Ref. [1], is actually a QOE, because its efficiency and its PWC are given by  $\eta = 1 - \nu_l / \nu_p$  and  $T_1 > (\nu_p / \nu_l) T_0$ , where  $\nu_l$  and  $\nu_p$  are the two energy gaps of the working substance, and  $T_1$  and  $T_0$  are the temperatures of the two heat baths, respectively.

### B. Classical versus quantum Otto engines

Below we prove that the operation efficiency  $\eta_O$  in Eq. (24) of a QOE, is also equal to the efficiency  $\eta_O^{\text{CL}}$  of a classical Otto engine. For simplicity, here we only consider a two-level system as the working substance (the result can be generalized to multilevel systems if all the eigenenergies of the multilevel system change in the same ratios as in the quantum adiabatic process [26]). For a two-level system (see Fig. 3), when the temperature  $T$  of the heat bath is fixed, the occupation probability  $P_e$  of the excited state  $|e\rangle$  in thermal equilibrium is a monotonically decreasing function of the level spacing  $\Delta$  between the two energy levels [3,12,13]. Its inverse function reads

$$\Delta_\theta = k_B T_\theta \ln \left( \frac{1}{P_e^\theta} - 1 \right), \quad \theta = h, l. \quad (26)$$

As mentioned above, the efficiency  $\eta_O$  in Eq. (24) of a QOE cycle represented by the rectangle ( $A$ - $B$ - $C$ - $D$ ) (see Fig. 3) is

$$\eta_O = 1 - \frac{\Delta_l}{\Delta_h}. \quad (27)$$

From Eqs. (26) and (27) and Fig. 3, we can see that the efficiency  $\eta_O$  of the QOE cycle can be rewritten as

$$\eta_O = 1 - \frac{T(C)}{T(B)} = 1 - \frac{T(D)}{T(A)}, \quad (28)$$

where  $T(i)$ , with  $i=A, B, C$ , and  $D$ , are the effective temperatures of the working substance at the instants  $A, B, C$ , and  $D$  indicated in Fig. 3. Here, we have used the relation  $\Delta(C)/\Delta(B) = T(C)/T(B)$  because of the fact  $P_e(C) = P_e(B) = P_e^h$  and Eq. (26), and similarly  $\Delta(D)/\Delta(A) = T(D)/T(A)$ . In the QOE cycle, the effective temperatures  $T(B)$  and  $T(D)$  of the working substance at instants  $B$  and  $D$  equal the temperatures of the two heat baths  $T(B) = T_h$ ,  $T(D) = T_l$ .

As for a classical Otto engine, the classical efficiency  $\eta_O^{\text{CL}}$  is [27]

$$\eta_O^{\text{CL}} = 1 - \left( \frac{V_h}{V_l} \right)^{\gamma-1}, \quad (29)$$

where  $V_l$  and  $V_h$  are the volumes of the classical ideal gas in the two classical isochoric processes (see Fig. 3), and  $\gamma$  is the classical adiabatic exponent [27]. Because  $TV^{\gamma-1}$  is constant during a classical adiabatic process, we can therefore eliminate the volumes in Eq. (29) as

$$\eta_O^{\text{CL}} = 1 - \frac{T_3}{T_2} = 1 - \frac{T_4}{T_1}, \quad (30)$$

where  $T_1, T_2, T_3$ , and  $T_4$  are the temperatures of the working substance at instants 1, 2, 3, and 4, and the temperatures at instants 2 and 4 are equal to the temperatures of the two heat baths  $T_2 = T_h$ ,  $T_4 = T_l$ . This is in very good agreement with the result of a QOE cycle in Eq. (28). Thus we proved that the efficiency of a QOE also equals its classical counterpart. Moreover, similar to Carnot engines, we plot the schematic temperature-entropy ( $T$ - $S$ ) diagrams for both a QOE cycle and a classical Otto engine cycle in Fig. 3(c). The similarity of the two  $T$ - $S$  diagrams also supports our definition of the QOE. Comparisons between the QOE and the classical Otto engine are listed in Table III.

### C. An alternative quantum Otto engine

Before concluding this section, we would like to revisit an alternative QOE cycle similar to that in Ref. [28] and that given most recently in [18]. As illustrated in Fig. 4, we consider two two-level systems (two qubits) as the working substance, which are denoted by qubit  $S$  and qubit  $D$ , and the level spacings of the two qubits are  $\Delta_S$  and  $\Delta_D$ , respectively. The temperatures of the two heat baths are  $T_S$  and  $T_D$ . Without loss of generality, here we choose  $T_S > T_D$  and  $\Delta_S > \Delta_D$ .

TABLE III. Quantum Otto engine versus classical Otto engine. Here ‘‘CIC’’ and ‘‘CA’’ refer to ‘‘classical isochoric processes’’ and ‘‘classical adiabatic processes,’’ respectively; ‘‘QIC’’ and ‘‘QA’’ refer to ‘‘Quantum isochoric processes’’ and ‘‘Quantum adiabatic processes,’’ respectively. Also,  $V_h$  and  $V_l$  are the volumes of the working substance (classical ideal gas) in the two classical isochoric processes;  $\gamma$  is the classical adiabatic exponent [27].  $T(i)$  ( $i=A, B, C, D$ ) and  $T_k$  ( $k=1, 2, 3, 4$ ) are defined in Fig. 3.

	Strokes	Efficiency	Positive-work condition
Classical	CIC-CA-CIC-CA	$\eta_O^{CL} = 1 - \left(\frac{V_h}{V_l}\right)^{\gamma-1} = 1 - \frac{T(C)}{T(B)} = 1 - \frac{T(D)}{T(A)}$	$T_h > T_l \left(\frac{V_l}{V_h}\right)^{\gamma-1}$
Quantum	QIC-QA-QIC-QA	$\eta_O = 1 - \frac{\Delta_l}{\Delta_h} = 1 - \frac{T_3}{T_2} = 1 - \frac{T_4}{T_1}$	$T_h > T_l \left(\frac{\Delta_h}{\Delta_l}\right)$

The alternative QOE cycle consists of two steps: (1) let the two qubits decouple from each other and contact their own heat baths, respectively, until they reach thermal equilibrium with these two heat baths; and (2) switch on the interaction between the two qubits and implement a SWAP operation between them. These two steps are shown in Figs. 4(a) and 4(b). The density matrices of the two qubits after step (1) are

$$\rho_i(1) = \frac{1}{Z_i} [ |0\rangle_i \langle 0|_i + \exp(-\beta_i \Delta_i) |1\rangle_i \langle 1|_i ] \quad (i = S, D), \quad (31)$$

where  $\beta_i = 1/k_B T_i$ , and for simplicity we have chosen the eigenenergy of the ground state as a reference point. After step (2), the density matrices become

$$\begin{aligned} \rho_S(2) &= \frac{1}{Z_D} [ |0\rangle_S \langle 0|_S + \exp(-\beta_D \Delta_D) |1\rangle_S \langle 1|_S ], \\ \rho_D(2) &= \frac{1}{Z_S} [ |0\rangle_D \langle 0|_D + \exp(-\beta_S \Delta_S) |1\rangle_D \langle 1|_D ]. \end{aligned} \quad (32)$$

After these two steps, the two qubits are decoupled and put into contact with their own bath, and a new cycle starts.

The key point of this alternative QOE cycle is that the

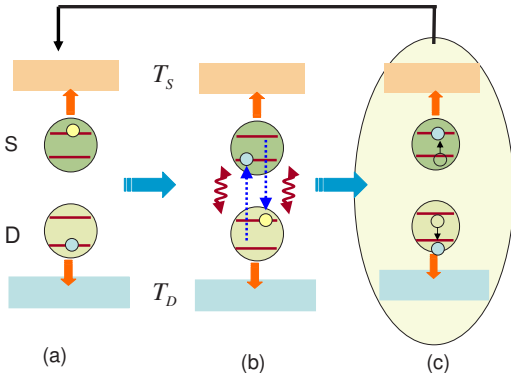


FIG. 4. (Color online) A schematic diagram illustrating an alternative quantum Otto engine. This QOE cycle consists of two steps: a SWAP between the two two-level systems (two qubits), shown in (b), and a thermalization with their respective heat baths, shown in (a). Step (c) indicates the transition from (b) to (a). The SWAP operation in (b) replaces the two quantum isochoric processes in the QOE cycle mentioned in the text and shown in Fig. 3(a).

SWAP operation takes place of the two quantum adiabatic processes, while the thermalization process takes place of two quantum isochoric processes. We can now calculate the heat absorbed by the qubit  $S$  and heat released by the qubit  $D$  in step (1),

$$\begin{aligned} Q_{in} &= \text{Tr}[H\rho_S(1)] - \text{Tr}[H\rho_S(2)] \\ &= \Delta_S \left( \frac{1}{Z_S} \exp(-\beta_S \Delta_S) - \frac{1}{Z_D} \exp(-\beta_D \Delta_D) \right), \end{aligned} \quad (33)$$

$$\begin{aligned} Q_{out} &= \text{Tr}[H\rho_D(2)] - \text{Tr}[H\rho_D(1)] \\ &= \Delta_D \left( \frac{1}{Z_S} \exp(-\beta_S \Delta_S) - \frac{1}{Z_D} \exp(-\beta_D \Delta_D) \right). \end{aligned} \quad (34)$$

The operation efficiency  $\eta$  of the QHE cycle can be calculated straightforwardly,

$$\eta = \frac{Q_{in} - Q_{out}}{Q_{in}} = 1 - \frac{\Delta_D}{\Delta_S}, \quad (35)$$

and the PWC is  $T_S > (\Delta_S/\Delta_D)T_D$ . Thus, this two-step cycle is an alternative QOE cycle. We will revisit, in more detail, this alternative QOE cycle in Sec. VII.

Let us here mention an alternative QCE of two qubits based on a SWAP operation. This alternative QCE cycle consists of three steps: (1) let the two qubits decouple and contact their own heat baths and both experience quantum isothermal processes, (2) switch on the interaction between the two qubits and implement a SWAP operation, and (3) let the two qubits decouple from each other and also decouple the two qubits from their heat baths, and subject them to a quantum adiabatic process. A similar QOE cycle and a QCE cycle have been studied in Ref. [28], where the SWAP operation was decomposed into three controlled-NOT (CNOT) operations.

## V. RELATIONS BETWEEN QUANTUM OTTO AND QUANTUM CARNOT CYCLES

In this section we discuss the relation between a quantum Otto engine cycle and a quantum Carnot engine cycle. For simplicity, here we use a two-level system as an example of working substance. Our results about QHEs based on a two-level system can be generalized to multilevel systems if all the eigenenergies of the multilevel system change by the same ratios in the quantum adiabatic processes [26].



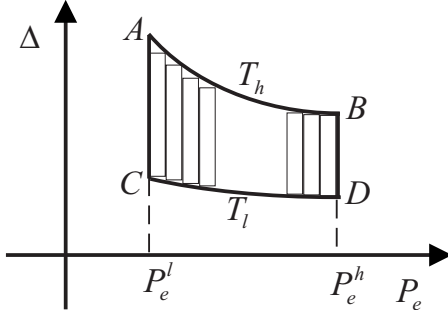


FIG. 5. A quantum Carnot engine cycle can be modeled as an infinite number of small quantum Otto engine cycles. Here,  $P_e^h$ ,  $P_e^l$ ,  $A$ ,  $B$ ,  $C$ ,  $D$ , and  $T_h$ ,  $T_l$  are defined in Fig. 2(a). The small rectangles inside the QCE cycle ( $A$ - $B$ - $C$ - $D$ ) represent small QOE cycles. The temperatures of the two heat baths of these QOE cycles are  $T_h$  and  $T_l$ , respectively, which are the same as that of the QCE cycle. For similar discussions see also Refs. [3,13,15,16].

### A. Quantum Carnot cycle derived from quantum Otto cycles

A QCE cycle can be decomposed into an infinite number of small QOE cycles (see Fig. 5) [3,13,15,16]. Now we give a concise and explicit proof about this observation. The heat absorbed and released in the infinite number of infinitesimal QOE cycles can be integrated by applying Eqs. (21), (22), and (26),

$$Q_{\text{in}} = T_h \int_{P_e^l}^{P_e^h} \ln(P_e^{-1} - 1) dP_e, \quad (36)$$

$$Q_{\text{out}} = T_l \int_{P_e^l}^{P_e^h} \ln(P_e^{-1} - 1) dP_e. \quad (37)$$

Then we obtain the positive work  $W$  done during the infinite number of infinitesimal QOE cycles ( $A$ - $B$ - $C$ - $D$ ) by making use of Eq. (23),

$$W = Q_{\text{in}} - Q_{\text{out}} = (T_h - T_l) \int_{P_e^l}^{P_e^h} \ln(P_e^{-1} - 1) dP_e. \quad (38)$$

From Eqs. (36) and (38) we can see that the efficiency of an infinite number of infinitesimal QOE cycles is

$$\eta = \frac{W}{Q_{\text{in}}} = 1 - \frac{T_l}{T_h}. \quad (39)$$

This is the efficiency of the QCE in Eq. (18). Thus we have proved that a QCE cycle can be modeled as an infinite number of infinitesimal QOE cycles. However, a finite QCE cycle and a finite QOE cycle cannot be equivalent because one is reversible and the other one is not. When the two cycles become infinitesimal, they can be infinitesimally close to each other.

### B. Quantum Otto cycle derived from quantum Carnot cycles

Conversely, a QOE cycle can also be modeled as an infinite number of QCE cycles (see Fig. 6), but the temperatures of the two heat baths of these small QCE are different. The

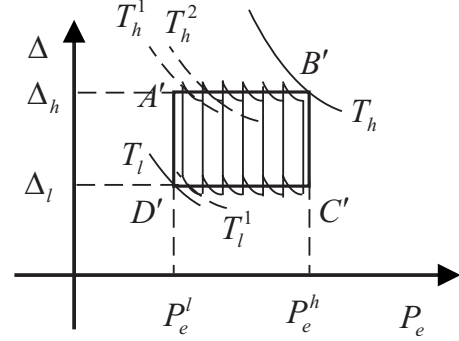


FIG. 6. A quantum Otto engine cycle can be modeled as an infinite number of small quantum Carnot engine cycles. Here  $P_e^h$ ,  $P_e^l$ ,  $T_h$ , and  $T_l$  are defined in Fig. 3(a). The small cycles inside the QOE cycle  $A'$ - $B'$ - $C'$ - $D'$  represent small quantum Carnot cycles. The temperatures of the two heat baths (e.g.,  $T_h^1$  and  $T_l^1$ ) of these small QCE cycles are different from that ( $T_h$  and  $T_l$ ) of the QCE cycle.

quantum isochoric process  $A' \rightarrow B'$  ( $C' \rightarrow D'$ ) can be modeled as many small quantum isothermal processes with temperatures  $T_h^1$  ( $T_l$ ),  $T_h^2$  ( $T_l^1$ ),  $T_h^3$  ( $T_l^2$ ), ... (see Fig. 6),

$$T_h^1 < T_h^2 < T_h^3 < \dots < T_h^N < T_h, \quad (40)$$

$$T_l < T_l^1 < T_l^2 < \dots < T_l^{N-1} < T_l^N. \quad (41)$$

The heat absorbed and released in the infinite number of infinitesimal QCE cycles can be obtained by applying  $dQ = TdS$  and Eq. (26),

$$Q_{\text{in}} = \int_{P_e^l}^{P_e^h} \frac{\Delta_h}{k_B} \frac{1}{\ln(P_e^{-1} - 1)} dS = \Delta_h \int_{P_e^l}^{P_e^h} dP_e, \quad (42)$$

$$Q_{\text{out}} = \int_{P_e^l}^{P_e^h} \frac{\Delta_l}{k_B} \frac{1}{\ln(P_e^{-1} - 1)} dS = \Delta_l \int_{P_e^l}^{P_e^h} dP_e, \quad (43)$$

where we have used the relation  $dS = -k_B[\ln P_e - \ln(1 - P_e)]dP_e$ . We then obtain the positive work  $W$  done during the infinite number of infinitesimal QCE cycles ( $A'$ - $B'$ - $C'$ - $D'$  in Fig. 6) by making use of Eq. (17),

$$W = Q_{\text{in}} - Q_{\text{out}} = (\Delta_h - \Delta_l)(P_e^h - P_e^l). \quad (44)$$

From Eqs. (42) and (44) we can see that the efficiency of an infinite number of infinitesimal QCE cycles is

$$\eta = \frac{W}{Q_{\text{in}}} = 1 - \frac{\Delta_l}{\Delta_h}. \quad (45)$$

This is the efficiency of the QOE in Eq. (27). Thus we have proved that a QOE cycle can be modeled as infinite number of infinitesimal QCE cycles.

We would like to mention that the formula  $dQ = TdS$  is applicable in Eq. (42) due to the fact that these infinite number of infinitesimal QCE cycles (with heat bath temperatures  $T_h^1$ ,  $T_l^1$ ;  $T_h^2$ ,  $T_l^2$ ; ...) are thermal equilibrium (reversible) processes since the entropy increase vanishes during these cycles (see Appendix C). However, if we take the QOE cycle as a whole, and the heat bath temperatures are  $T_h$  and  $T_l$ , this process is a nonequilibrium (irreversible) process. Hence, the

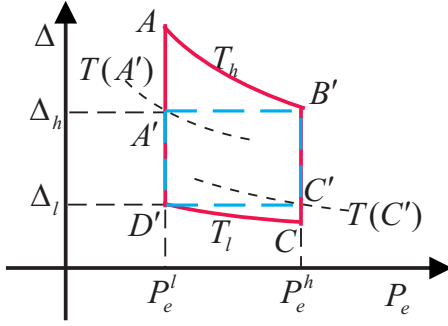


FIG. 7. (Color online) Schematic diagrams for a quantum Carnot engine cycle ( $AB'CD'$  red continuous line) and a quantum Otto engine cycle ( $A'B'C'D'$  blue dashed line) based on a two-level system. Here, points  $B'$  and  $D'$  are the same for both cycles. The temperatures  $T_h$  and  $T_l$  of the two heat baths of the two QHE cycles and the occupation probabilities  $P_e^h$  and  $P_e^l$  in two quantum adiabatic processes are the same. The net work done during a cycle is proportional to the area enclosed by the four curves which represent the cycles.

formula  $dQ=TdS$  is not applicable here. This is why we cannot apply Eqs. (14) and (15) in calculating  $Q_{in}^{QIC}$  and  $Q_{out}^{QIC}$  in the QOE cycle in Sec. IV A.

### C. Comparison of work and efficiency for quantum Otto and quantum Carnot cycles

Having clarified the properties of the QCE and QOE, here we now compare the thermodynamic properties of a QCE cycle with that of a QOE cycle and study the relation between them. For the two QHE cycles (QCE cycle and QOE cycle), we consider the case with the same heat baths (at high and low temperatures  $T_h$  and  $T_l$ , respectively), and the same occupation probabilities ( $P_e^h$  and  $P_e^l$ , respectively) in the two quantum adiabatic processes (see Fig. 7).

First, let us compare the amounts of positive work done in a QCE cycle and a QOE cycle under the same conditions defined above. The positive work done during the QCE cycle (here denoted by  $A-B'-C-D'$  in Fig. 7) can also be written as

$$W_C = \int_{P_e^l}^{P_e^h} [\Delta(T_h, P_e) - \Delta(T_l, P_e)] dP_e, \quad (46)$$

while the work done during a QOE cycle is (here denoted by  $A'-B'-C'-D'$  in Fig. 7)

$$W_O = \int_{P_e^l}^{P_e^h} (\Delta_h - \Delta_l) dP_e. \quad (47)$$

From Fig. 7 we know for any  $P_e \in [P_e^l, P_e^h]$ , we have  $\Delta(T_h, P_e) - \Delta(T_l, P_e) > \Delta_h - \Delta_l$ . Hence, from Eqs. (46) and (47) we have  $W_C > W_O$ ; i.e., under the same conditions, the work done during a QCE cycle is more than that during a QOE cycle.

Next we consider the efficiencies of the QCE cycle and the QOE cycle under the same conditions. From Eq. (27) we know that the efficiency of a small QOE cycle can be rewritten as

$$\begin{aligned} \eta_O &= 1 - \frac{k_B T_l \ln[(P_e^l)^{-1} - 1]}{k_B T_h \ln[(P_e^l)^{-1} - 1]} \\ &\approx 1 - \frac{T_l}{T_h} \left\{ 1 - \frac{\partial}{\partial P_e} \left[ \ln \ln \left( \frac{1}{P_e} - 1 \right) \right] (P_e^h - P_e^l) \right\} \\ &= \eta_C + \frac{T_l}{T_h} \frac{\partial}{\partial P_e} \left[ \ln \ln \left( \frac{1}{P_e} - 1 \right) \right] (P_e^h - P_e^l). \end{aligned} \quad (48)$$

It can be verified that the second term on the right-hand side (RHS) of Eq. (48) is negative. Thus we have proved the inequality

$$\eta_O = 1 - \frac{\Delta_l}{\Delta_h} < 1 - \frac{T_l}{T_h} = \eta_C \quad (49)$$

for every small cycle. We conclude that, under the same conditions, the QCE is more efficient than the QOE, even for any finite cycle.

## VI. ILLUSTRATIONS OF QUANTUM CARNOT ENGINE AND QUANTUM OTTO ENGINE

As mentioned above, to construct a multilevel (including two-level) Carnot-type QHE, two preconditions (mathematical results) are required: (1) all energy gaps change by the same ratio in the quantum adiabatic process (when the working substance performs work); (2) the ratio of the energy gap changes in the quantum adiabatic process should equal the ratio of the temperatures of the two heat baths, so that the thermodynamic cycle is reversible. Physically, these two conditions can always be satisfied for a QHE based on a two-level system, because there is only one energy gap in a two-level system, we can always find a proper effective temperature to characterize the working substance. Besides the two-level system, the harmonic oscillator and a particle confined in an infinite square well potential are two other examples that can illustrate the basic properties of the QCE and the QOE. This is because in both cases all energy gaps change by the same ratio when changing the parameters of the system, and we can always use a proper effective temperature to characterize the working substance in the quantum adiabatic process, too. Below we calculate the amount of positive work done during a thermodynamic cycle using those working substances.

### A. Two-level systems

Let us now consider a QHE based on a two-level system, e.g., a spin- $\frac{1}{2}$  system in an external magnetic field pointing along the  $+z$  direction, the Hamiltonian of the working substance is

$$H_{\text{TLS}}(i) = -MB(i)(|\uparrow\rangle\langle\uparrow| - |\downarrow\rangle\langle\downarrow|), \quad (50)$$

where  $B(i)$  is the strength of the external field at instant  $i$ ,  $i = A, B, C, D$  (see Fig. 2 and Fig. 3);  $M = e\hbar/2mc$  is the Bohr magnon;  $|\downarrow\rangle$  and  $|\uparrow\rangle$  indicate the spin-down (excited) state and spin-up (ground) state, respectively. The thermal equilibrium state can be written as

TABLE IV. Comparison of several properties of quantum Otto engines and quantum Carnot engines using the following *quantum* substances as working substances: Two-level system (TLS), harmonic oscillator (HO), and a particle confined in an infinite square (IS) potential. The operation efficiency  $\eta$ , the positive-working condition (PWC), and the amount of work  $W$  extracted in a thermodynamic cycle are listed (see Sec. VI).

		Two-level system (TLS)	Harmonic oscillator (HO)	Infinite square well (IS)
Quantum Otto engine	$\eta_O$	$1 - \frac{\Delta_l}{\Delta_h}$	$1 - \frac{\omega_l}{\omega_h}$	$1 - \left(\frac{L_l}{L_h}\right)^2$
	PWC	$T_h > \frac{\Delta_h}{\Delta_l} T_l$	$T_h > \frac{\omega_h}{\omega_l} T_l$	$T_h > \left(\frac{L_h}{L_l}\right)^2 T_l$
	$W_O$	$W_O^{\text{TLS}}$	$W_O^{\text{HO}}$	$W_O^{\text{IS}}$
Quantum Carnot engine	$\eta_C$	$1 - \frac{T_l}{T_h}$	$1 - \frac{T_l}{T_h}$	$1 - \frac{T_l}{T_h}$
	PWC	$T_h > T_l$	$T_h > T_l$	$T_h > T_l$
	$W_C$	$W_C^{\text{TLS}}$	$W_C^{\text{HO}}$	$W_C^{\text{IS}}$

$$\rho_{\text{TLS}}(i) = \frac{1}{Z(i)} \{ \exp[\beta_i MB(i)] |\uparrow\rangle\langle\uparrow| + \exp[-\beta_i MB(i)] |\downarrow\rangle\langle\downarrow| \}, \quad (51)$$

where  $Z(i) = \exp[\beta_i MB(i)] + \exp[-\beta_i MB(i)]$  is the partition function at instant  $i$ . Applying Eq. (16) we obtain the entropy of the working substance

$$S^{\text{TLS}}(i) = k_B \ln[Z(i)] + k_B \beta_i MB(i) \tanh[\beta_i MB(i)]. \quad (52)$$

Then from Eqs. (14), (15), and (17) we obtain the net work done by the working substance during a QCE cycle,

$$W_C^{\text{TLS}} = (T_h - T_l)[S^{\text{TLS}}(B) - S^{\text{TLS}}(A)]. \quad (53)$$

The net work done during the QOE cycle can be calculated by applying Eq. (23),

$$W_O^{\text{TLS}} = (\Delta_h - \Delta_l) \left( \frac{1}{1 + \exp(\beta_h \Delta_h)} - \frac{1}{1 + \exp(\beta_l \Delta_l)} \right). \quad (54)$$

Another example of QHE based on a two-level system is a photon-Carnot engine [5,6,11]. After performing a similar calculation we recover the operation efficiency  $1 - T_l/T_h$  in Eq. (18) and the PWC  $T_h > T_l$ . Hence, this photon-Carnot engine is actually a two-level QCE.

### B. Harmonic oscillator

For a QHE based on a harmonic oscillator with the eigenenergies  $E_n(i) = (n - 1/2)\hbar\omega(i)$ , by applying Eq. (16), we derive the entropy  $S^{\text{HO}}(i)$  of the working substance as

$$S^{\text{HO}}(i) = -k_B \ln\{1 - \exp[-\beta_i \hbar\omega(i)]\} + k_B \beta_i \hbar\omega(i) \frac{1}{\exp[\beta_i \hbar\omega(i)] - 1}, \quad (55)$$

and the work done during a QCE cycle as

$$W_C^{\text{HO}} = (T_h - T_l)[S^{\text{HO}}(B) - S^{\text{HO}}(A)]. \quad (56)$$

The net work done during the QOE cycle can be obtained by applying Eq. (23),

$$W_O^{\text{HO}} = \hbar(\omega_h - \omega_l) \left( \frac{1}{\exp(\beta_h \hbar\omega_h) - 1} - \frac{1}{\exp(\beta_l \hbar\omega_l) - 1} \right). \quad (57)$$

### C. Particle in an infinite square potential well

For a QHE based on a particle confined in an infinite square (IS) potential, the eigenenergies are  $E_n(i) = \gamma_i n^2$ , where  $\gamma_i = (\pi\hbar)^2 / (2mL_i^2)$ ;  $m$  and  $L_i$  are the mass of the particle and the width of the square well at instant  $i$ , respectively. The entropy of the working substance can also be calculated by applying Eq. (16),

$$S^{\text{IS}}(i) = \frac{k_B}{2} + k_B \ln\left(\frac{1}{2} \sqrt{\frac{\pi}{\beta_i \gamma_i}}\right). \quad (58)$$

In obtaining Eq. (58) we make an approximation

$$\sum_{n=1}^{\infty} \exp(\gamma_i n^2) \approx \int_0^{\infty} \exp(\gamma_i n^2) dn. \quad (59)$$

So the work done during a QCE cycle can be expressed as (17),

$$W_C^{\text{IS}} = (T_h - T_l)[S^{\text{IS}}(B) - S^{\text{IS}}(A)], \quad (60)$$

while the net work done during a QOE cycle is (23),

$$W_O^{\text{IS}} = \frac{\pi}{8} (\gamma_h - \gamma_l) \left( \frac{1}{(\beta_h \gamma_h)^2} - \frac{1}{(\beta_l \gamma_l)^2} \right). \quad (61)$$

In order to better compare the results, they are all listed in Table IV.

Before concluding this section, we would like to mention that, our current QHE model can only be implemented with

quantum systems with all energy levels being discrete (all eigenstates being bound states). Besides the harmonic oscillator and the infinite square well system, we can find other potentials that satisfy discrete spectral structure requirement to implement our QHE. However, we cannot deal with quantum systems with continuous spectral structure, e.g., a particle in a Coulomb potential or a finite square well. We will extend our current study to quantum systems with continuous spectral structure in future research.

## VII. MAXWELL'S DEMON AND QUANTUM OTTO ENGINE

In the above discussions, we give clear definitions of microscopic QCE and QOE cycles through clarifying the basic quantum thermodynamic processes (e.g., quantum isochoric process and quantum isothermal process). These results indicate that the properties, such as the operation efficiency, of macroscopic (classical) heat engines can be obtained from the microscopic (quantum) level as long as we clarify the basic thermodynamic processes microscopically. In the previous discussions, our QCE and QOE models show no contradiction with the thermodynamic laws.

In one of our recent studies [18], we proposed a Maxwell's demon-assisted quantum thermodynamic cycle to study the function of a Maxwell's demon, and we also studied how it affects the second law of thermodynamics. It is interesting that when the restoration of the demon is properly included into the QHE cycle, the efficiency of the Maxwell's demon assisted QHE cycle has the same form as that for a QOE derived previously in Eq. (27). Hence, the apparent violation of the second law due to Maxwell's demon is prevented. In this section, we also would like to study the intrinsic relation between these two kinds of quantum thermodynamic cycles. We would also like to add some details about the Maxwell's demon-assisted quantum thermodynamic cycle proposed in Ref. [18] to better demonstrate our main idea.

### A. Maxwell's demon erasure not included in the thermodynamic cycle

We first analyze a single-reservoir thermodynamic cycle with external control based on the effective temperature defined above. It can be proved that the property of this cycle is similar to that of the QHE cycle proposed in Ref. [18]. Our thermodynamic cycle consists of three steps: (1) quantum rotation, (2) decoherence, and (3) thermalization.

After the thermalization process, the state of the two-level system (with the ground state  $|0\rangle$ , the excited state  $|1\rangle$  and the level spacing  $\Delta$ ) can be described by a density matrix

$$\rho(0) = P_1|1\rangle\langle 1| + P_0|0\rangle\langle 0|, \quad (62)$$

where the probability distributions  $P_1$  and  $P_0$  in the two-level system are determined by the temperature  $T_l$  of the heat reservoir and the level spacing  $\Delta$ . Then, the two-level system, driven by an external field (we do not treat it as a part of the system for the moment), undergoes a rotation,

$$|1\rangle \rightarrow |\tilde{1}\rangle = \cos \theta |1\rangle + \sin \theta |0\rangle,$$

$$|0\rangle \rightarrow |\tilde{0}\rangle = -\sin \theta |1\rangle + \cos \theta |0\rangle. \quad (63)$$

If the time interval of this rotation is much shorter than the relevant time of the thermalization, the state  $\rho(0)$  of the two-level system becomes

$$\rho(1) = P'_1|1\rangle\langle 1| + P'_0|0\rangle\langle 0| + \text{ODT}, \quad (64)$$

where

$$P'_1 = P_1 \cos^2 \theta + P_0 \sin^2 \theta, \\ P'_0 = P_1 \sin^2 \theta + P_0 \cos^2 \theta, \quad (65)$$

and ODT denotes the off-diagonal terms, which disappear rapidly (pure dephasing) due to the coupling between the two-level system and the reservoir. Actually two effects (dephasing and dissipation) occur when the two-level system is coupled to the reservoir [29]. The first process occurs much faster than the second one, and thus we can consider the two effects separately. After considering dephasing (but before considering dissipation), the state  $\rho(1)$  of the two-level system becomes

$$\rho(2) = P'_1|1\rangle\langle 1| + P'_0|0\rangle\langle 0|. \quad (66)$$

This state is obviously not in equilibrium with respect to the reservoir at temperature  $T_l$ . But we can imagine there is such a reservoir at temperature  $T_h$ , which can be expressed as

$$T_h(P_0, P_1, \theta) = \frac{\Delta}{k_B} \ln^{-1} \left( \frac{P_1 \sin^2 \theta + P_0 \cos^2 \theta}{P_1 \cos^2 \theta + P_0 \sin^2 \theta} \right). \quad (67)$$

This effective temperature  $T_h(P_0, P_1, \theta)$  possesses some exotic features. For example, when  $\theta = \pi/2$ ,  $P'_1 = P_0$ , and  $P'_0 = P_1$ . This means that  $T_h = -T_l$  is a "negative temperature" since there exists a population inversion  $P'_1 \geq P'_0$ . Only when  $P'_0 > P'_1$ ,  $T_h$  is positive. Finally, the two-level system is put into contact with the heat bath for a sufficiently long time. After the thermalization process, the state  $\rho(2)$  returns to  $\rho(0)$ , and a thermodynamic cycle is finished and the two-level system seems to extract work from a single heat bath. We can imagine it as a thermodynamic cycle between two reservoirs with the temperature  $T_l$  and a virtual temperature  $T_h$ . Actually contradictions to the second law can appear due to this "negative temperature."

It is not surprising that the above result (a contradiction to the second law) appears since we do not include the controller for the rotation operators shown in Eq. (63). This result is very similar to those single-particle heat engines assisted by a classical Maxwell's demon proposed by Szilard.

Now, let us describe a new version of Szilard single-particle heat engine (see Fig. 8). The working substance of the QHE is a spin (two-level system) with ground state  $|0\rangle$ , and excited state  $|1\rangle$ . The level spacing is  $\Delta$ . We first put the two-level system into a heat bath at temperature  $T$ . After a sufficiently long thermalization process, the spin reaches a thermal equilibrium state, which can be described by  $\rho(0)$ , similarly defined as above. Second, a demon performs a



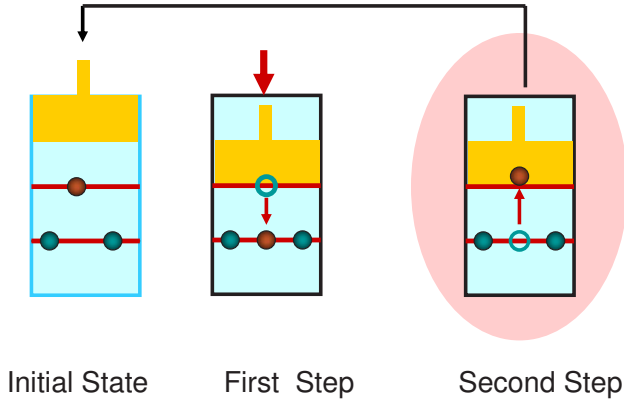


FIG. 8. (Color online) Schematic diagram of the two-level version of the Szilard single-particle heat engine. An invisible demon detects the state of the two-level working substance and then controls it to do work: when the system is in the excited state, the demon makes the working substance flip to the ground state (the first step); when the system is in the ground state, the demon does nothing for the working substance. After these operations the working substance is brought in contact with a very large heat bath and then thermalized into its initial state (the second step).

measurement. If the measurement result is confirmed that the system is in its upper state, then the spin is flipped and positive work is done by the spin with an amount  $\Delta$ . If the measurement result confirms that the system is in its lower state, then no work is done. Then the system is put into contact with the heat bath and a new cycle starts. This is a two-step Maxwell's demon-assisted QHE. A similar discussion has been given in Ref. [3]. It is easy to see that the net effect of this QHE is to absorb heat from a single heat bath and convert it into work. On average, the net work done per cycle is  $P_1\Delta$ . This is a perpetual machine of the second kind. This apparent violation of the second law is seen because the erasure of the demon is not included into the QHE cycle.

### B. Maxwell's demon erasure included in the thermodynamic cycle

In Ref. [18], we have demonstrated that, when the erasure of the information stored in the Maxwell's demon is considered into the QHE cycle, the apparent violation of the second law does not hold. That is, there is no violation of the second law even in the existence of such Maxwell's demon.

To show the above observation, let us consider in more detail a thermodynamic cycle including the Maxwell's demon (see the Fig. 9). Let us explain each step of the QHE cycle proposed in Ref. [18]. First, two qubits (two-level systems)  $S$  and  $D$  are decoupled and separately coupled to two heat baths with different temperatures  $T_S$  and  $T_D$ . After a period of time longer than both the dephasing time  $T_2$  and the relaxation time  $T_1$ , they are thermalized to two equilibrium states  $\rho_S(1)$  and  $\rho_D(1)$ ,

$$\rho_F(1) = P_F^1|1\rangle\langle 1| + P_F^0|0\rangle\langle 0|, \quad (68)$$

for  $F=S$  and  $D$ , respectively. The joint thermalized state  $\rho(1) = \rho_S(1) \otimes \rho_D(1)$  of the total system with  $S$  plus  $D$  can be written as

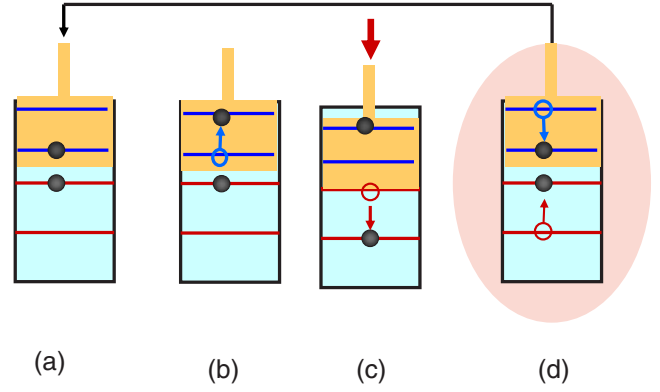


FIG. 9. (Color online) Schematic illustration for the Maxwell's demon-assisted quantum heat engine with four steps: (a) Both the QHE of the two-level system and a demon is hidden in the "piston" as another two-level system is initialized in thermal equilibrium states with different temperatures; (b) the demon makes a quantum nondemolition measurement about the state of the two-level system  $S$  with a CNOT operation: when  $S$  is seen in the excited state it records this information through a transition from its ground state to the excited state; when  $S$  is in its ground state, the demon remains in its original state; (c) according to the information recorded by the demon, the demon can enable the system to operate through another CNOT logical gate: If the demon was encoded in the excited state it will make the system flip; otherwise it enables the system to remain; (d) both the system and the demon are brought into contact with their own heat baths and then thermalized with different temperatures from their own initial states, respectively. During this process, the information stored in the demon is totally erased and the entire system completes a quantum thermodynamic cycle.

$$\begin{aligned} \rho(1) = & P_{S,D}^{1,1}|1,1\rangle\langle 1,1| + P_{S,D}^{1,0}|1,0\rangle\langle 1,0| + P_{S,D}^{0,1}|0,1\rangle\langle 0,1| \\ & + P_{S,D}^{0,0}|0,0\rangle\langle 0,0|, \end{aligned} \quad (69)$$

where we have defined the direct product of the eigenstate of the two qubits

$$|q,q'\rangle \equiv |q\rangle_S \otimes |q'\rangle_D \quad (q,q' = 0,1), \quad (70)$$

and the joint probabilities  $P_{S,D}^{q,q'} \equiv P_S^q P_D^{q'}$ .

Second, two consecutive unitary operations: a CNOT operation flipping the demon states only when the working substance system is in its excited state [28], and the demon controls the system to do work. Physically, the system experiences a conditional evolution (CEV). The changes of the states in the two operations can be expressed as follows:

$$\begin{aligned} |0,0\rangle & \xrightarrow{\text{CNOT}} |0,0\rangle \xrightarrow{\text{CEV}} |0,0\rangle, \\ |0,1\rangle & \xrightarrow{\text{CNOT}} |0,1\rangle \xrightarrow{\text{CEV}} |\tilde{0},1\rangle, \\ |1,0\rangle & \xrightarrow{\text{CNOT}} |1,1\rangle \xrightarrow{\text{CEV}} |\tilde{1},1\rangle, \\ |1,1\rangle & \xrightarrow{\text{CNOT}} |1,0\rangle \xrightarrow{\text{CEV}} |1,0\rangle, \end{aligned} \quad (71)$$

where  $|\tilde{0}\rangle$  and  $|\tilde{1}\rangle$  are defined in Eq. (63). These two subprocesses can be realized with two quantum nondemolition Hamiltonians

$$H_{\text{CNOT}} = H_{S \rightarrow D}, \quad H_{\text{CEV}} = H_{D \rightarrow S}, \quad (72)$$

where

$$H_{A \rightarrow B} = \frac{\mathcal{E}}{4} (1 + \sigma_Z^A) \otimes \sigma_X^B \quad (73)$$

is a typical CEV Hamiltonian with  $A$  controlling  $B$ . It produces a time evolution of the system  $B$  as a quantum rotation defined by Eq. (63) with  $\theta = gt$ , when the system  $A$  is initially prepared in  $|1\rangle_A$ . Here,  $\sigma_j^F$ ,  $F=A, B$  ( $j=x, y, z$ ), are the Pauli matrices of the two-level system  $A$  and  $B$ . Obviously the CNOT operation on the demon is given by the time evolution produced by  $H_{\text{CNOT}}$  with  $\theta = \pi/2$ .  $H_{\text{CNOT}}$  performs a quantum nondemolition measurement of the state of the working substance  $S$ .

After this CNOT operation, the density matrix changes from  $\rho(1)$  to

$$\begin{aligned} \rho(2) &= \text{CNOT}\{\rho(1)\} \\ &= P_{S,D}^{1,1}|1,0\rangle\langle 1,0| + P_{S,D}^{1,0}|1,1\rangle\langle 1,1| + P_{S,D}^{0,1}|0,1\rangle\langle 0,1| \\ &\quad + P_{S,D}^{0,0}|0,0\rangle\langle 0,0|. \end{aligned} \quad (74)$$

From Eq. (74) we can derive the reduced density matrices  $\rho_S(2)$  and  $\rho_D(2)$  of the working substance and the demon

$$\rho_S(2) = \text{Tr}_D[\rho(2)] = \rho_S(1) \quad (75)$$

and

$$\rho_D(2) = \text{Tr}_S[\rho(2)] = (p_{S,D}^{1,1} + p_{S,D}^{0,0})|0\rangle\langle 0| + (p_{S,D}^{1,0} + p_{S,D}^{0,1})|1\rangle\langle 1|, \quad (76)$$

respectively. During this process, the system  $S$  remains in its initial state while the demon acquires information. Meanwhile, the internal energy changes at the expense of using an amount of work  $W_D$ ,

$$W_D = \text{Tr}[H\rho_D(2)] - \text{Tr}[H\rho_D(1)] = \Delta_D(P_D^1 - P_{S,D}^{1,0} - P_{S,D}^{0,1}). \quad (77)$$

From Eqs. (69) and (74) we see that the total entropy of  $S$  and  $D$  does not change during the CNOT operation

$$\begin{aligned} S(2) &= -k_B(P_{S,D}^{1,1} \ln P_{S,D}^{1,1} + P_{S,D}^{1,0} \ln P_{S,D}^{1,0} + P_{S,D}^{0,1} \ln P_{S,D}^{0,1} \\ &\quad + P_{S,D}^{0,0} \ln P_{S,D}^{0,0}) \\ &= -k_B(P_S^1 \ln P_S^1 + P_S^0 \ln P_S^0) - k_B(P_D^1 \ln P_D^1 + P_D^0 \ln P_D^0) \\ &\equiv S_S(1) + S_D(1) \equiv S(1). \end{aligned} \quad (78)$$

Hence, our model verifies the prediction in Refs. [33,34] that a measurement does not necessarily lead to entropy increase. Also, we know from Eq. (75) that the entropy of  $S$  during the CNOT operation does not change,

$$S_S(2) = S_S(1). \quad (79)$$

But the entropy of  $D$  changes as

$$\begin{aligned} \delta S_D &= S_D(2) - S_D(1) \\ &= -k_B[(P_{S,D}^{1,1} + P_{S,D}^{0,0}) \ln(P_{S,D}^{1,1} + P_{S,D}^{0,0}) + (P_{S,D}^{1,0} \\ &\quad + P_{S,D}^{0,1}) \ln(P_{S,D}^{1,0} + P_{S,D}^{0,1})] + k_B(P_D^1 \ln P_D^1 + P_D^0 \ln P_D^0). \end{aligned} \quad (80)$$

We would like to point out that the mutual entropy

$$S_M(2) = S_D(2) + S_S(2) - S(2) = S_D(2) - S_D(1) \quad (81)$$

does not vanish (it vanishes before this CNOT operation). And this nonvanishing mutual entropy can be used to measure the information acquired by the demon about the system [30].

Next we consider the changes of entropy and energy after the quantum control (the CEV) process. The state of the demon and the working system after the CEV is

$$\rho(3) = \text{CEV}\{\rho(2)\}, \quad (82)$$

and then,

$$\begin{aligned} \rho(3) &= P_{S,D}^{1,1}|1,0\rangle\langle 1,0| + P_{S,D}^{1,0}|\tilde{1},1\rangle\langle \tilde{1},1| + P_{S,D}^{0,1}|\tilde{0},1\rangle\langle \tilde{0},1| \\ &\quad + P_{S,D}^{0,0}|0,0\rangle\langle 0,0|. \end{aligned} \quad (83)$$

The reduced density matrices of the working substance  $\rho_S(3)$  and the demon  $\rho_D(3)$  are, respectively,

$$\begin{aligned} \rho_S(3) = \text{Tr}_D[\rho(3)] &= P_{S,D}^{1,0}|\tilde{1}\rangle\langle \tilde{1}| + P_{S,D}^{0,1}|\tilde{0}\rangle\langle \tilde{0}| + P_{S,D}^{1,1}|1\rangle\langle 1| \\ &\quad + P_{S,D}^{0,0}|0\rangle\langle 0| \end{aligned} \quad (84)$$

and

$$\rho_D(3) = \text{Tr}_S[\rho(3)] = \rho_D(2). \quad (85)$$

Similarly, the energy change (work performed by the working system) during this process is

$$\begin{aligned} W_S &= \text{Tr}[H\rho_S(2)] - \text{Tr}[H\rho_S(3)] \\ &= \Delta_S(P_S^1 - P_{S,D}^{1,1} - P_{S,D}^{1,0}|\langle \tilde{1}|1\rangle|^2 - P_{S,D}^{0,1}|\langle \tilde{0}|1\rangle|^2). \end{aligned} \quad (86)$$

In particular, when we choose  $\theta = \pi/2$ , the CEV is a CNOT, and the reduced density matrix of  $S$  can be written as

$$\rho_S(3) = P_D^1|1\rangle\langle 1| + P_D^0|0\rangle\langle 0|, \quad (87)$$

and the entropy of the system is

$$S_S(3) = -k_B(P_D^1 \ln P_D^1 + P_D^0 \ln P_D^0) \equiv S_D(1).$$

So the change of the entropy of the working substance in the CEV process is

$$\delta S_S = S_S(3) - S_S(2) = S_D(1) - S_S(1), \quad (88)$$

where we have used Eq. (79). But from Eqs. (78), (82), and (85), we know that both the total entropy of  $S$  plus  $D$  and the entropy of the demon  $D$  do not change, i.e.,

$$S(1) = S(2) = S(3),$$

$$S_D(3) = S_D(2). \quad (89)$$

Finally,  $S$  and  $D$  are decoupled and put into contact with their own baths, and a new cycle starts. In the thermalization process, no work is done, but heat is exchanged between the

heat baths and  $S$  and  $D$ . The thermalization process is an information-erasure process. This kind of zero-work erasure with a low temperature reservoir was first introduced in Ref. [31], and studied afterwards in Ref. [32]. In the thermalization process the heat absorbed by  $S$  is

$$Q_{\text{in}} = \text{Tr}[H\rho_S(1)] - \text{Tr}[H\rho_S(3)] \\ = \Delta_S(P_{S,D}^{1,0} - P_{S,D}^{0,1})|\langle\tilde{1}|1\rangle|^2 - P_{S,D}^{0,1}|\langle\tilde{0}|1\rangle|^2, \quad (90)$$

and the heat released by the demon  $D$  is

$$Q_{\text{out}} = \text{Tr}[H\rho_D(3)] - \text{Tr}[H\rho_D(1)] = \Delta_D(P_{S,D}^{1,0} + P_{S,D}^{0,1} - P_D^1). \quad (91)$$

Now we include the erasure of the memory of Maxwell's demon into the thermodynamic cycle, and we will show that, under certain conditions, our composite QHE is equivalent to a simple QOE.

For each cycle described above, we are now able to calculate the work  $W$  performed by the heat engine

$$W = W_S - W_D = \Delta_S(P_{S,D}^{1,0} - P_{S,D}^{0,1})|\langle\tilde{1}|1\rangle|^2 - P_{S,D}^{0,1}|\langle\tilde{0}|1\rangle|^2 \\ - \Delta_D(P_{S,D}^{1,0} - P_{S,D}^{0,1}). \quad (92)$$

It can be checked that in the thermodynamic cycle  $W = Q_{\text{in}} - Q_{\text{out}}$ . This is just the first law of thermodynamics. The positive-work condition can be derived from Eq. (92),

$$T_S \geq T_D \left( \frac{\Delta_D}{\Delta_S} \right). \quad (93)$$

Notice that when we choose the CEV to be the special case  $\theta = \pi/2$  (i.e., a CNOT), the heat absorbed  $Q_{\text{in}}$  and positive work  $W$  done during a cycle can be simplified to

$$Q_{\text{in}} = \Delta_S(P_{S,D}^{1,0} - P_{S,D}^{0,1}), \quad (94)$$

$$W = \Delta_S(P_{S,D}^{1,0} - P_{S,D}^{0,1}) - \Delta_D(P_{S,D}^{1,0} - P_{S,D}^{0,1}), \quad (95)$$

and

$$\eta = \frac{W}{Q_{\text{in}}} = 1 - \frac{\Delta_D(P_{S,D}^{1,1} - P_{S,D}^{1,0})}{\Delta_S(P_{S,D}^{1,0} - P_{S,D}^{0,1})}. \quad (96)$$

If we further assume the temperature  $T_D$  to be so low that  $\exp(-\beta_D \Delta_D) \ll 1$ , i.e., the demon is "erased" nearly to its ground state  $\rho_D(1) \approx |0_D\rangle\langle 0_D|$  (the zero-entropy "standard state" was also discussed in Refs. [31–33]). Then the efficiency of our QHE, Eq. (96), becomes

$$\eta = 1 - \frac{\Delta_D}{\Delta_S}. \quad (97)$$

This is the efficiency of a simple QOE cycle without Maxwell's demon, as shown in Eq. (27). Otherwise the operation efficiency in Eq. (96) is less than the efficiency of a simple QOE cycle. This is because (i) among all CEV's, the CNOT is the optimal operation to extract work, and (ii) when  $T_D$  is vanishingly small, the demon can be restored to a zero-entropy "standard state" to acquire information about the system in the most efficient way.

## VIII. CONCLUSIONS AND REMARKS

By defining the quantum version of basic thermodynamic processes, we study the basic properties of a QCE. To construct a QCE cycle, two preconditions about the quantum adiabatic process are required: first, all energy gaps of the working substance must change by the same ratio, such as in harmonic oscillators and infinite square well potentials. Second, the change of the ratio of the energy gaps must equal the ratio of the temperatures of the two heat baths. We find that the working efficiency for the QCE is the same as that of the classical Carnot engine though the internal energy may change in the quantum isothermal process. We also study the properties of the QOE and compare these with the classical Otto engine, and we find that the efficiency and positive-work condition are the same when expressed in terms of temperatures (see Table III). Through comparing the thermodynamic cycles of the two QHEs, we clarify the relationship between them, and we demonstrate that the QCE (QOE) cycle can be modeled as an infinite number of small QOE (QCE) cycles. We also discuss some experimentally realizable physical systems that can be used to implement our QHE. Finally, through a generalized QOE, we demonstrate that there is no violation of the second law, even when there is a Maxwell's demon. This is a prediction of Landauer's principle [34–38].

Before concluding this paper, we want to emphasize three points. First, in our present study the working substance is always assumed to be in a thermal equilibrium state, and quantum coherence is not considered here, our study is not related with the result that the efficiency of a QHE is less than its classical counterpart  $\eta_Q \leq \eta_C$ , as in Ref. [28]. Second, we only consider the quasistatic process. Hence, the time intervals of these processes are infinitely long and the output power is vanishingly small. Recently, finite-time QHE cycles [15,39] (nonzero output power) and frictionlike behavior [16] of the QOE were studied, where the increase of power occurs at the expense of decreasing operation efficiency. Third, we will further extend our current study to QHE with quantum-many-body system as the working substance. In this extended case, we will consider the quantum statistical effects, e.g., the Bose-Einstein condensation, of the working substance. We believe these quantum effects will advance our understanding of the relation between quantum mechanics and thermodynamics and bring important insights into some fundamental problems in quantum thermodynamics.

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**APPENDIX A: INVARIANCE UNDER ENERGY SHIFT**

The amount of positive work  $W_O$  done during a QOE cycle remains invariant under the uniform shift of all energy levels. If we shift all the energy levels  $E_n^l$  in Fig. 1,

$$\tilde{E}_n^l = E_n^l - \delta, \quad (\text{A1})$$

the amount of work done during a QOE cycle becomes

$$\tilde{W}_O = \sum_n (P_n^h - \tilde{P}_n^l)(E_n^h - \tilde{E}_n^l),$$

where  $\tilde{P}_n^l$  are the occupation probabilities after the energy levels are shifted. It is easy to find that the occupation probabilities  $\tilde{P}_n^l$  remain invariant under such an energy shift

$$\tilde{P}_n^l = e^{-(E_n^l - \delta)\beta_l} \left( \sum_n e^{-(E_n^l - \delta)\beta_l} \right)^{-1} = e^{-E_n^l \beta_l} \left( \sum_n e^{-E_n^l \beta_l} \right)^{-1} = P_n^l. \quad (\text{A2})$$

Thus, after the energy levels shift, the net work  $\tilde{W}_O$  done during a QOE cycle can be simplified to

$$\tilde{W}_O = \sum_n (P_n^h - P_n^l)(E_n^h - E_n^l + \delta) = \sum_n (P_n^h - P_n^l)(E_n^h - E_n^l), \quad (\text{A3})$$

which is just the net work  $W_O$  done by the working system during a QOE cycle before the level shift. Similarly we can prove that  $W_O$  remains invariant under the shift  $\tilde{E}_n^h = E_n^h - \delta$ .

Following the same way we can prove that other properties of the QHE, such as operation efficiency and positive work conditions, are invariant under uniform shift of all energy levels as well. Hence, we can simply assume the eigenenergy of the ground state to be zero  $E_0^h = E_0^l = 0$ . This energy shift is convenient for our discussion about QHE later. This result can be easily generalized to any QCE cycle, because in Sec. V, we demonstrate that a QCE can be modelled as an infinite number of small QOE cycles.

**APPENDIX B: INTERNAL ENERGY OF THE WORKING SUBSTANCE IN QUANTUM ISOTHERMAL PROCESSES**

The internal energy of a system is

$$U(i) = \text{Tr}[\rho(i)H(i)]. \quad (\text{B1})$$

In an isothermal expansion process, all energy levels change in the same ratio

$$E_n \rightarrow \zeta E_n, \quad n = 0, 1, 2, \dots,$$

where  $\zeta$  is the ratio of energy levels and  $0 < \zeta < 1$ . When the energy levels change, the internal energy of the system can be rewritten as

$$U(\zeta) = \sum_n \frac{\zeta E_n}{Z(\zeta)} \exp(-\beta_h \zeta E_n), \quad (\text{B2})$$

where

$$Z(\zeta) = \sum_n \exp(-\beta_h \zeta E_n) \quad (\text{B3})$$

is the partition function. To test whether the internal energy of the system is invariant under the change of energy levels, we take the derivative

$$\begin{aligned} \frac{dU(\zeta)}{d\zeta} &= \sum_n \frac{E_n}{Z(\zeta)} (1 - \zeta \beta_h E_n) \exp(-\beta_h \zeta E_n) \\ &+ \zeta \beta_h \left( \sum_n \frac{E_n}{Z(\zeta)} \exp(-\beta_h \zeta E_n) \right)^2. \end{aligned} \quad (\text{B4})$$

For two-level systems, there is only one term in the sum over  $n$ , because we assume the eigenenergy of the ground state to be zero. Thus Eq. (B4) can be simplified as

$$\frac{dU(\zeta)}{d\zeta} = \frac{E_e}{Z(\zeta)} \exp(-\beta_h \zeta E_e) \left( 1 - \frac{\zeta \beta_h E_e}{Z(\zeta)} \right), \quad (\text{B5})$$

where  $E_e$  is the eigenenergy of the excited state of the two-level system. The RHS of Eq. (B5) is obviously nonzero.

For a harmonic oscillator with the eigenfrequency  $\omega$ , we assume the eigenenergy of the ground state to be zero (neglecting the ground-state energy  $\hbar\omega/2$ ), then Eq. (B4) can be simplified to

$$\frac{dU(\zeta)}{d\zeta} = - \left( \frac{\hbar\omega(\beta_h \zeta \hbar\omega - 1)}{\exp(\beta_h \zeta \hbar\omega) - 1} \right) - \beta_h \zeta \left( \frac{\hbar\omega}{\exp(\beta_h \zeta \hbar\omega) - 1} \right)^2. \quad (\text{B6})$$

The RHS of Eq. (B6) is obviously nonzero.

For a particle confined in an infinite square potential,  $E_n = \gamma n^2$ , where  $\gamma$  has been defined in Eq. (58). Then Eq. (B4) can be simplified to

$$\begin{aligned} \frac{dU(\zeta)}{d\zeta} &= \sum_n \frac{\gamma n^2 - \beta_h \zeta \gamma^2 n^4}{Z(\zeta)} \exp(-\beta_h \zeta \gamma n^2) \\ &+ \beta_h \zeta \left( \sum_n \frac{\gamma n^2}{Z(\zeta)} \exp(-\beta_h \zeta \gamma n^2) \right)^2, \end{aligned} \quad (\text{B7})$$

where

$$Z(\zeta) = \sum_n \exp(-\beta_h \zeta \gamma n^2) \quad (\text{B8})$$

is the partition function. We make an approximation

$$Z(\zeta) \approx \int_0^\infty \exp(-\beta_h \zeta \gamma n^2) dn = \frac{1}{2} \sqrt{\frac{\pi}{\beta_h \zeta \gamma}}, \quad (\text{B9})$$

and then Eq. (B7) can be simplified to

$$\frac{dU(\zeta)}{d\zeta} = 0. \quad (\text{B10})$$

The RHS of Eq. (B10) is zero. Hence, we conclude that in an isothermal process, the derivation of the internal energy over the energy levels in Eq. (B4) is not always zero. Accordingly, the internal energy of the system may vary with the change of the energy levels.



**APPENDIX C: THERMODYNAMIC REVERSIBILITY  
OF AN INFINITE NUMBER OF INFINITESIMAL  
QUANTUM ISOTHERMAL PROCESSES**

We consider a two-level system interacting with a heat bath. The temperature of the heat bath is well controlled so that the two-level system is always in thermal equilibrium with the heat bath. Now let us calculate the entropy (von Neumann entropy) increase in the two-level system and the entropy (thermodynamic entropy) decrease in the heat bath. We assume the two-level system initially in thermal equilibrium with a heat bath at the temperature  $T_h^1$  [see Eq. (40) and Fig. 6], and finally the temperature of the heat bath is controlled to increase to  $T_h$  (see Fig. 6). The entropy of the initial state of the system at  $A'$  (see Fig. 6) is

$$\begin{aligned} S_{\text{TLS}}(A') &= -k_B \{ \Lambda'_- \exp(-\Delta_h \beta'_h) \\ &\quad \times \ln[\Lambda'_- \exp(-\Delta_h \beta'_h)] + \Lambda'_+ \ln \Lambda'_+ \} \\ &= \frac{\Delta_h}{T_h^1} \Lambda'_+ - k_B \ln[\Lambda'_+ \exp(\Delta_h \beta'_h)], \end{aligned} \quad (\text{C1})$$

where  $\beta'_h = 1/(k_B T_h^1)$  and

$$\begin{aligned} \Lambda'_\pm &= \frac{1}{1 + \exp(\pm \Delta_h \beta'_h)}, \\ \Lambda_\pm &= \frac{1}{1 + \exp(\pm \Delta_h \beta_h)}. \end{aligned} \quad (\text{C2})$$

Similarly, we obtain that the entropy of the final state of the two-level system at  $B'$  (see Fig. 6) is

$$S_{\text{TLS}}(B') = \frac{\Delta_h}{T_h} \Lambda_+ - k_B \ln[\Lambda_+ \exp(\Delta_h \beta_h)]. \quad (\text{C3})$$

So the entropy increase of the two-level system in the infinite number of infinitesimal quantum isothermal processes ( $A' \rightarrow B'$  in Fig. 6) is

$$\begin{aligned} dS_{\text{TLS}} &= S_{\text{TLS}}(B') - S_{\text{TLS}}(A') \\ &= \frac{\Delta_h}{T_h} \Lambda_+ - k_B \ln[\Lambda_+ \exp(\Delta_h \beta_h)] \\ &\quad - \left( \frac{\Delta_h}{T_h^1} \Lambda'_+ - k_B \ln[\Lambda'_+ \exp(\Delta_h \beta'_h)] \right). \end{aligned} \quad (\text{C4})$$

Next we calculate the entropy decrease of the heat bath in the same process. The thermodynamic entropy decrease of the heat bath due to its coupling to the two-level system can be expressed as

$$\begin{aligned} dS_{\text{Bath}} &= \int_{T_h^1}^{T_h} \frac{\Delta_h dp_e}{T} \\ &= k_B \int_{T_h^1}^{T_h} \left[ (\Lambda_+)^2 \left( \frac{\Delta_h}{k_B} \right)^2 - (\Lambda_+)^2 \left( \frac{\Delta_h}{k_B} \right)^2 \right] \frac{dT}{T}. \end{aligned} \quad (\text{C5})$$

We apply the transformation

$$\begin{aligned} T &= \frac{\Delta_h}{k_B \ln t}, \\ dT &= \frac{\Delta_h}{k_B} \left( -\frac{1}{\ln^2 t} \right) \frac{dt}{t}. \end{aligned} \quad (\text{C6})$$

Under this transformation  $dS_{\text{Bath}}$  (C5) can be further given as

$$\begin{aligned} dS_{\text{Bath}} &= k_B \left[ \left( \frac{\ln t}{1+t} \right) \Big|_{\exp(\Delta_h \beta'_h)}^{\exp(\Delta_h \beta_h)} - \ln \left( \frac{t}{1+t} \right) \Big|_{\exp(\Delta_h \beta'_h)}^{\exp(\Delta_h \beta_h)} \right] \\ &= \frac{\Delta_h}{T_h} \Lambda_+ - k_B \ln[\Lambda_+ \exp(\Delta_h \beta_h)] \\ &\quad - \left( \frac{\Delta_h}{T_h^1} \Lambda'_+ - k_B \ln \Lambda'_+ \exp(\Delta_h \beta'_h) \right). \end{aligned} \quad (\text{C7})$$

From Eqs. (C4) and (C7) we can see that  $dS_{\text{Bath}} = dS_{\text{TLS}}$ , i.e., the entropy decrease in the bath is equal to the entropy increase in the two-level system. Thus we have proved that the total entropy is conserved in these infinite number of infinitesimal quantum isothermal processes, and these processes are thermodynamically reversible.

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