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Quantum thermodynamic cycles and quantum heat engines (II)

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We study the quantum mechanical generalization of pressure or force, and then we extend the classical thermodynamic isobaric process to quantum mechanical system. Based on these efforts, we are able to study the quantum version of thermodynamic cycles that consist of quantum isobaric process, such as Brayton cycle and Diesel cycle. We also consider the implementation of quantum Brayton cycle and quantum Diesel cycle with some example systems, such as single particle in 1D box and single-mode radiation field. These studies lay the microscopic (quantum mechanical) foundation for Szilard-Zurek single molecule engine.

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I. INTRODUCTION

Quantum thermodynamics is the study of heat and work dynamics in quantum mechanical systems [1]. In the extreme limit of small systems with only a few degrees of freedom, both the small size and quantum effects influence the thermodynamic properties dramatically [2–4]. The interplay between thermodynamics and quantum physics has been a interesting research topic since 1950s [5]. In recent years, with the developments of nanotechnology and experimental technique, the study of the interface between quantum physics and thermodynamics begins to attract more and more attention [7]. Studies of quantum thermodynamics not only have important potential applications in nanotechnology and quantum information processing, but also bring new insights onto some fundamental problems of thermodynamics, such as Maxwell's demon and the universality of the second law [6]. Among all the studies of quantum thermodynamics, a central concern is to make quantum mechanical extension of classical thermodynamic processes and cycles [8].

It is well know that in classical thermodynamics, there are four basic thermodynamic processes: adiabatic process, isothermal processes, isochoric process, and isobaric process [9]. These four processes correspond to constant entropy, constant temperature, constant volume, and constant pressure, respectively. From these four basic thermodynamic processes, we can construct all kinds of thermodynamic cycles, such as Carnot cycle, Otto cycle, Brayton cycle, et al [10]. Among all the four kinds of basic thermodynamic processes, quantum version of adiabatic process – quantum adiabatic process – has been extensively studied ever since the born of quantum mechanics, while no attention has been paid to the quantum mechanical generalization of the remaining three basic thermodynamic processes for decades. In recent years the development of quantum thermodynamics renews the interests of quantum thermodynamics processes. In a recent paper [8], one (HTQ) of us and collaborators systematically study the quantum mechanical generalization of the isothermal and the isochoric process. Base on these studies, the properties of quantum Carnot cycle and quantum Otto cycle are clarified. Numerous studies on other quantum thermodynamic cycles are also reported [11]. However, as to our best knowledge, the quantum mechanical generalization of isobaric process has not been studied systematically so far. Probably, the lack of the consideration of quantum isobaric process is due to the fact that "pressure" (force) [12] is not a well defined observable in a quantum mechanical system. Because of the short of a well defined quantum isobaric process, the quantum thermodynamic cycles that consist of quantum isobaric process, such as quantum Brayton cycle and quantum Diesel cycle, are not well studied.

In this paper, we will focus on the study of the quantum isobaric process [10] and its related quantum thermodynamic cycles. We will begin with the definition of "pressure" for an arbitrary quantum system, and then generalize the classical isobaric process to quantum mechanical system. After that we successfully establish the complete mapping between four basic thermodynamic processes and their quantum counterpart. Based on these generalizations of thermodynamic processes, we are able to study an arbitrary thermodynamic cycle constructed by any of these four thermodynamic processes. As an example, we will discuss the Brayton cycle and Diesel cycle and compare their properties with their classical counterpart. We notice that some discussions about quantum Brayton cycle have been reported before [13]. Nevertheless, we found that their definition of pressure is ambiguous, and in their studies they cannot bridge the quantum and classical thermodynamic cycles. On the contrary, we will see that our definition of pressure for a quantum system has clear physical implication and our study bridges the thermodynamic cycles for quantum and classical system. Comparisons between these quantum thermodynamic cycles and their classical counterpart enable us to extend our understanding of the thermodynamics at the interface of classical and quantum physics. This paper is organized as follows: In Sec. II, we define microscopically "pressure" for a quantum mechanical system and study quantum mechanical generalization of isobaric process; in Sec. III, we study quantum Brayton cycle and study how the efficiency of Brayton cycle bridges quantum and classical thermodynamic cycles; in Sec. IV we study quantum Diesel cycle in comparison with their classical counter part; Sec. V is the remarks and conclusion.

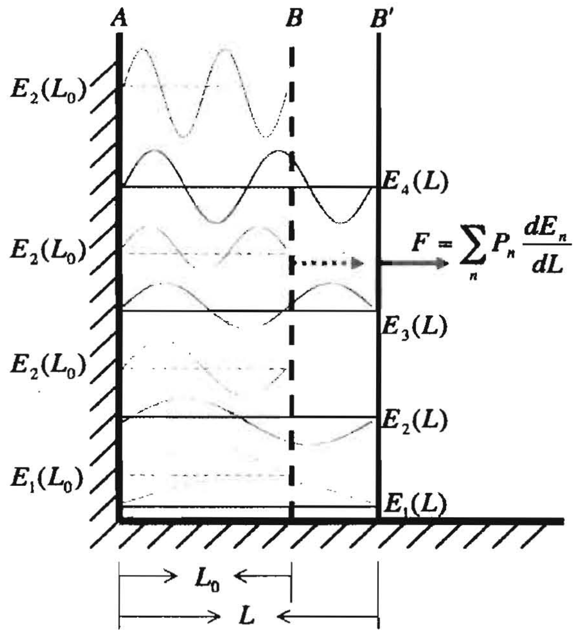

FIG. 1: Schematic diagram of pressure in quantum mechanical system (single particle in 1D box). One wall (A) of the square well is fixed, while the other one (B) is movable. The force acting on the wall B by the quantum system can be calculated from Eq. (3)

II. QUANTUM ISOBARIC PROCESS

A. Pressure in quantum-mechanical system

In order to study quantum isobaric process, we must first generalize pressure to an arbitrary quantum mechanical system. Let us recall that in some previous work [8, 14], heat and work have been generalized to quantum mechanical system, and the first law of thermodynamics has also been generalized to quantum mechanical systems.

$$\begin{aligned} \text{đ}Q &= \sum_n E_n dP_n, \\ \text{đ}W &= \sum_n P_n dE_n, \\ dU &= \text{đ}Q + \text{đ}W = \sum_n (E_n dP_n + P_n dE_n), \end{aligned} \tag{1}$$

where E_n is the nth eigenenergy of the quantum mechanical system with the Hamiltonian $H = \sum_n E_n |n\rangle \langle n|$ under consideration and P_n is the occupation probability in the nth eigenstate $\rho = \sum_n P_n |n\rangle \langle n|$; $|n\rangle$ is the nth eigenstate of the Hamiltonian; $\text{đ}Q$ and $\text{đ}W$ are the heat exchange and work done respectively during a thermodynamic process. From classical thermodynamics we know that the first law can be expressed as $dU = \text{đ}Q + \text{đ}W = TdS + \sum_n Y_n dy_n$. Here, T and S refer to temperature and entropy; Y_n is the generalized force and y_n is generalized coordinate (displacement under the generalized force) corresponding to Y_n [15]. Inversely, the generalized force can be expressed as

$$Y_n = -\frac{\text{đ}W}{dy_n}. \tag{2}$$

For example, when the generalized force is chosen to be the pressure P, and its corresponding generalized coordinate is the volume V, we have its corresponding pressure $P = -\text{đ}W/dV$. For a quantum mechanical system, e.g., a single particle in 1D box [16] (see Fig. 1), we can also define the force (generalized pressure) acting on either wall of the potential well. In this case, the generalized coordinate is the width L of the potential. Thus, from the definition of work (1) we have

$$F = -\frac{\text{đ}W}{dL} = -\sum_n P_n \frac{dE_n}{dL}. \tag{3}$$

This is the expression of pressure in quantum mechanical system. Alternatively, the expression of force (3) in a quantum mechanical system can be obtained in a statistical-mechanical way.

$$\begin{aligned} F &= -\left(\frac{\partial \mathbb{F}}{\partial L}\right)_T = kT\left(\frac{\partial \ln Z}{\partial L}\right)_T = kT\frac{1}{Z}\frac{\partial}{\partial L}\sum_n e^{-\beta E_n} \\ &= \sum_n \left(\frac{e^{-\beta E_n}}{Z}\right)\frac{\partial E_n}{\partial L} = \sum_n P_n \frac{\partial E_n}{\partial L}, \end{aligned} \tag{4}$$

where $\mathbb{F} = -kT \ln Z$ is the free energy of the quantum system, and $Z = \sum_n e^{-\beta E_n}$ is the partition function. When P_n satisfy Gibbs distribution $P_n = \frac{1}{Z}e^{-\beta E_n}$, or the system is in equilibrium, the expectation value F (3) should gives the usual force in classical thermodynamics. We will see later that if we consider a single-mode photon field in a cavity instead of a single particle in 1D box as the working substance, this definition of force agrees with the radiation pressure obtained in thermodynamics. Thus our definition of pressure (force) has clear physical implication. We would like to mention that the definition of force in (3) and (4) is a further step of quantum thermodynamics after the identification of heat and work (1), and we will see these definitions for a quantum mechanical system are self-consistent.

B. Quantum isobaric process

Having clarified force for a quantum mechanical system, in the following we will study how to extend classical isobaric process to a quantum mechanical system. Classical isobaric process is a thermodynamic process, in which the pressure of the system remains a constant. The relaxation time scale of the system with the heat bath is much shorter than the time scale at which we control the volume of the system [17]. Hence, we can always assume the system in equilibrium with the heat bath. In order to achieve a constant pressure during the isobaric process, we must carefully control the temperature of the system, i.e., carefully change the temperature of the heat bath when we change the volume of the classical system [10]. For example, in the isobaric process of classical idea gas, the temperature of the system are required to be proportional to the volume of the gas due to the equation of state of the classical ideal gas $P = nR\frac{T}{V}$. For a quantum mechanical system, however, the change of the temperature may not be so obvious as classical ideal gas. Let us consider the quantum isobaric process based on a single particle in 1D box. The energy spectrum of the system is $E_n(L) = (\pi\hbar n)^2/(2mL^2)$. Here, m is the mass of the particle, and L is the width of the potential well (see Fig. 1). For such a quantum mechanical system, the pressure on the wall (equation of state of the working substance) can be obtained from Eq. (3)

$$\begin{aligned} F &= -\sum_n P_n(L)\frac{dE_n(L)}{dL} \\ &= -\sum_n \frac{\exp[-\beta(L)E_n(L)]}{Z(L)}\frac{dE_n(L)}{dL} \\ &= -\sum_n \frac{\exp[-\beta(L)\frac{\pi^2\hbar^2n^2}{2mL^2}]}{\frac{1}{2}\sqrt{\frac{2mL^2}{\pi\hbar^2\beta(L)}}} \times \frac{(-2)}{L} \times \frac{\pi^2\hbar^2n^2}{2mL^2} \\ &= \frac{4}{L}\sqrt{\frac{\pi\hbar^2\beta(L)}{2mL^2}}\left[-\frac{\partial}{\partial\beta(L)}\sum_n \exp[-\beta(L)\frac{\pi^2\hbar^2n^2}{2mL^2}]\right] \\ &= \frac{4}{L}\sqrt{\frac{\pi\hbar^2\beta(L)}{2mL^2}}\left[-\frac{\partial}{\partial\beta(L)}\frac{1}{2}\sqrt{\frac{2mL^2}{\pi\hbar^2\beta(L)}}\right] \\ &= \frac{1}{L\beta(L)}, \end{aligned} \tag{5}$$

where $Z(L) = \sum_n \exp[-\beta(L)E_n(L)]$ is the width-dependent partition function. The above equation is equivalent to the equation of motion of "classical" one-particle gas [16]. That means if we want to keep the pressure as a constant, we must control the temperature of the system to be proportional to the width of the potential well when the system in the box push one of the walls to perform work. We would like to mention that the temperature function of the "volume" of the quantum mechanical system is system-dependent. I.e., for different systems, the function of the temperature over the "volume" differs from one to another.

In the following we consider a single-mode radiation field in a cavity as the working substance of a Brayton cycle, which is first proposed in Ref. [3]. We assume that the cavity of length L and cross-section A can support only a single mode of the field $\omega = \frac{s\pi c}{L}$, where s is an integer. The Hamiltonian of the system is equivalent to a quantum harmonic oscillator

$$H = \sum_n (n + \frac{1}{2})\hbar\omega \left|n\right\rangle \left\langle n\right|, \tag{6}$$

From Eq. (3) we know that the radiation force F can be expressed as the derivative of the work over the length of the cavity

$$\begin{aligned} F &= -\sum_n \frac{e^{-\beta(L)E_n(L)}}{Z(L)}\frac{dE_n(L)}{dL} \\ &= -\frac{1}{1-e^{-\beta(L)\hbar\omega}}\sum_n e^{-\beta(L)n\hbar\omega}\left[(n+\frac{1}{2})\hbar\omega\right]\frac{1}{L}, \\ &= \left[\frac{\hbar\omega}{e^{\beta(L)\hbar\omega}-1} + \frac{1}{2}\hbar\omega\right]\frac{1}{L} \end{aligned} \tag{7}$$

From Eq. (8) we know that in order to achieve a constant force, we must carefully control the temperature of the heat bath when the width of the cavity changes

$$\beta(L) = \frac{L}{\hbar s\pi c}\ln\frac{2FL^2 + \hbar s\pi c}{2FL^2 - \hbar s\pi c} \tag{8}$$

It can be seen that for the single-mode radiation field, the temperature function (8) is much more complicated than that (5) of 1D box system in a quantum isobaric process.

For the convenience of later analysis, we would also like to calculate the entropy and the internal energy of the two systems mentioned above. First we consider the single particle in 1D box. The entropy expression can be obtained from the above Eq. (1) and Eq. (58) of Ref. [8].

$$S(L) = k_B\left[\frac{1}{2} + \ln\left(\frac{1}{2}\sqrt{\frac{2mL^2}{\pi\hbar^2\beta(L)}}\right)\right] \tag{9}$$

Comparing with the entropy of classical ideal gas, we can find that the entropy of classical idea gas gives exactly the entropy of single-particle in 1D box if we choose $N = 1$. We plot the entropy-temperature diagram according to the explicit expression (9) (See Fig. 4). The internal energy of the single particle in 1D box during the isobaric process can also be obtained analytically. Because the system is always in thermal equilibrium with the time-dependent heat bath, we can obtain the internal energy

$$\begin{aligned} U(L) &= -\frac{\partial\ln Z(L)}{\partial\beta(L)} = -\frac{1}{Z(L)}\frac{\partial Z(L)}{\partial\beta(L)} \\ &= -2\sqrt{\frac{\pi\hbar^2\beta(L)}{2mL^2}} \times \frac{1}{2}\sqrt{\frac{2mL^2}{\pi\hbar^2\beta(L)}} \times \left(-\frac{1}{2}\right)\frac{1}{\beta(L)} \\ &= \frac{1}{2}\frac{1}{\beta(L)} \end{aligned} \tag{10}$$

This expression of internal energy verifies the equipartition theorem [9]. Here we justified the result in Ref. [8] again: the internal energy of the infinite square potential system depends only on the temperature. From Eq. (9) and (10) we see that both the entropy and the internal energy of 1D box system has the same form as that of classical ideal gas. Moreover, from Eq. (5) we know that 1D box system has the same equation of state as that of classical ideal gas. Thus we conclude that 1D box system is the quantum mechanical counter part of classical ideal gas. This is basis of the discussion of Szilard-Zurek single molecule engine [16].

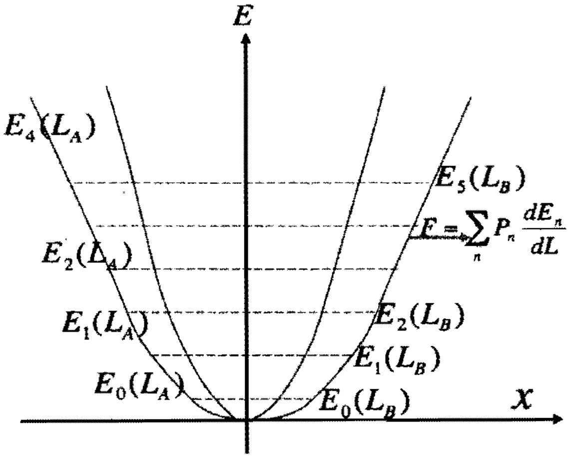

FIG. 2: Isobaric process based on single-mode radiation field (a quantum harmonic oscillator). Here the width of the potential $L \propto \frac{1}{\omega}$. $E_n(L_\alpha)$, $\alpha = A, B$ are the nth eigenenergy of the single mode radiation field with the potential width equals to L_α.

Similarly, let us consider the entropy and internal energy of single-mode radiation field. The entropy and the internal energy can also be calculated as that in Ref. [3]

$$S(L) = \frac{\langle n \rangle \hbar\omega}{T} + k \ln(\langle n \rangle + 1) \tag{11}$$

where $\langle n \rangle = [\exp(\hbar\omega/kT) - 1]^{-1}$ is the mean photon number, and the internal energy

$$U(L) = \sum_n \frac{e^{-\beta n \hbar\omega}}{Z(L)}(n + \frac{1}{2})\hbar\omega = (\langle n \rangle + \frac{1}{2})\hbar\omega \tag{12}$$

It is not difficult to find that the entropy (11) and the internal energy (12) of a single mode radiation field have different form from that of a single particle in 1D box system (9-10) , or from classical ideal gas. The internal energy (12) of single mode radiation field depends on both the temperature and the width of the potential well. In addition, the equation of state (7) of the single mode radiation field differ from from that (5) of single particle in 1D system, or classical ideal gas. Based on these observations, we say that the single mode radiation field has total different thermodynamic properties from that classical ideal gas. It can be inferred that in contrast to quantum heat engine based on single particle in 1D box, which is the quantum mechanical counter part of classical ideal gas, quantum heat engine based on single mode radiation field can give us new results beyond that of classical ideal gas.

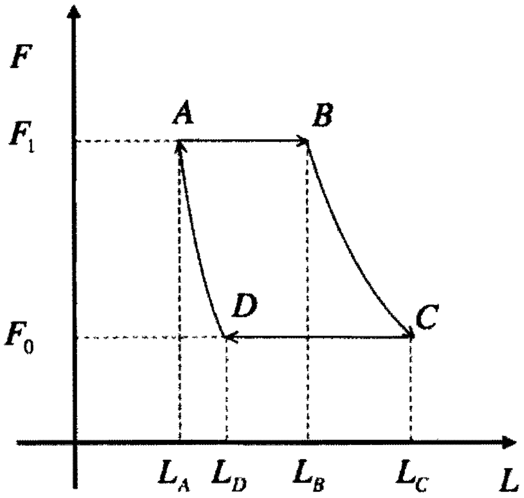

FIG. 3: Force-Displacement (Pressure-Volume) $F - L$ diagram of a quantum Brayton cycle based on a single particle in 1D box or single mode radiation field. $A \longrightarrow B$ represents an isobaric expansion process with a constant force F_1; $B \longrightarrow C$ represents an adiabatic expansion process with constant entropy S_1; $C \longrightarrow D$ represents an isobaric compression process with constant pressure F_0; $D \longrightarrow A$ is another adiabatic compression process with constant entropy S_0.

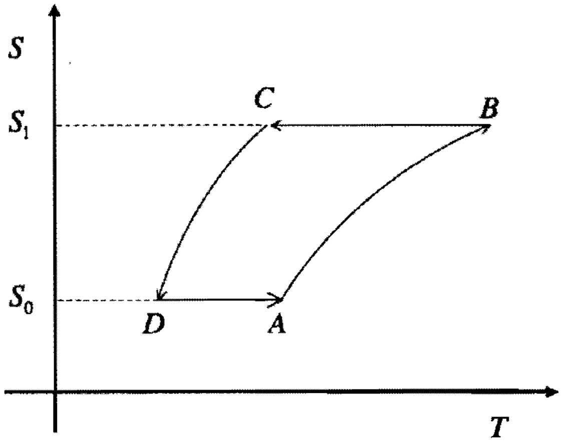

FIG. 4: Temperature-Entorpy $T - S$ diagram of Brayton cycle (see Fig. 3). In two adiabatic processes, $B \longrightarrow C$ and $D \longrightarrow A$ the entropy remains a constant.

III. QUANTUM BRAYTON CYCLE

In last section, we successfully extend the classical isobaric process to quantum mechanical system based on the definition of pressure (3) in a quantum mechanical system. In this section and next section, we will study two kinds of thermodynamic cycles consisting of quantum isobaric processes, and compare them with their classical counterpart. We first consider a quantum Brayton cycle based on a single particle in 1D box, and compare it with a classical Brayton cycle. A quantum Brayton cycle is an quantum mechanical analogue of classical Brayton cycle, which consists of two quantum isobaric processes and two quantum aidabatic processes. Similar to or previous work, we give a $T - S$ diagram of the quantum Brayton cycle (See Fig. 4). According to our definition of heat exchange in quantum mechanical system (1), we obtain the heat absorbed by the system from a time-dependent heat bath during the quantum isobaric expansion process $A \longrightarrow B$

$$\begin{aligned}
\text{đ}Q_{AB} =& \int_{L_A}^{L_B} \left[\sum_n E_n(L) \frac{dP_n(L)}{dL} \right] dL \\
=& \sum_n \int_{L_A}^{L_B} \left[[E_n(L)P_n(L)]' - \frac{dE_n(L)}{dL} P_n(L) \right] dL \\
=& \sum_n [E_n(L_B)P_n(L_B) - E_n(L_A)P_n(L_A)] \\
&+ \int_{L_A}^{L_B} F(L) dL \\
=& \frac{1}{2}[F_1 L_B - F_1 L_A] + F_1(L_B - L_A) \\
=& \frac{3}{2} F_1 (L_B - L_A).
\end{aligned} \tag{13}$$

Similarly, we can obtain the heat released to the time-dependent low temperature entropy sink

$$\text{đ}Q_{CD} = \frac{3}{2} F_0 (L_C - L_D). \tag{14}$$

Hence, the efficiency of the quantum Brayton cycle based on a single particle in 1D box can be expressed as

$$\eta = 1 - \frac{F_0(L_C - L_D)}{F_1(L_B - L_A)}. \tag{15}$$

Due to the equation of motion (5) and (10) $F_1 L_B / 2 = U(L_B)$, $F_0 L_C / 2 = U(L_C)$, and the relation of internal energy in the quantum adiabatic process $B \longrightarrow C$

$$\frac{U(L_B)}{U(L_C)} = \left(\frac{L_C}{L_B} \right)^2, \tag{16}$$

we have

$$\frac{F_1}{F_0} = \left(\frac{L_C}{L_B} \right)^3 \tag{17}$$

for the quantum adiabatic process $B \longrightarrow C$. Through a similar analysis we obtain

$$\frac{F_1}{F_0} = \left(\frac{L_D}{L_A} \right)^3 \tag{18}$$

for another quantum adiabatic process. Based on the above result (15), (17), and (18), we obtain the efficiency

$$\eta = 1 - \left(\frac{F_0}{F_1} \right)^{\frac{2}{3}}. \tag{19}$$

From Eq. (9) we know that in quantum adiabatic process ($S = const$), we have $TL^2 = const$. As a result the adiabatic exponent $\gamma = 3$ is obtained through comparison with $TL^{\gamma - 1} = const$ for adiabatic process. We would like to mention that in classical Brayton cycle, the efficiency of a classical Brayton cycle is $\eta = 1 - \left(\frac{F_0}{F_1} \right)^{1 - \frac{1}{\gamma}}$ [10], where γ is the classical adiabatic exponent. Thus our study bridges the quantum Brayton cycle and classical Brayton cycle by the efficiency (19) and the adiabatic exponent ($\gamma = 3$). Hence our definition of pressure for a quantum mechanical system is self-consistent.

In the following we consider a Brayton cycle based on a single-mode radiation fieldd. Similar to the above analysis, we calculate the heat absorbed by the system during the quantum isobaric expansion process $A \longrightarrow B$ (see Fig. 3)

$$\begin{aligned}
\text{đ}Q_{AB} =& \int_{L_A}^{L_B} \left[\sum_n E_n(L) \frac{dP_n(L)}{dL} \right] dL \\
=& [U(L_B) - U(L_A)] + \int_{L_A}^{L_B} F d(L) \\
=& \left(\frac{\hbar\omega_B}{e^{\beta(L_B)\hbar\omega_B} - 1} + \frac{\hbar\omega_B}{2} \right) \\
&- \left(\frac{\hbar\omega_A}{e^{\beta(L_A)\hbar\omega_A} - 1} + \frac{\hbar\omega_A}{2} \right) + F_H(L_B - L_A) \\
=& F_1(L_B - L_A),
\end{aligned} \tag{20}$$

where we have used the identity in the quantum isobaric process ($A \longrightarrow B$)

$$F_1 \equiv \frac{U(L_A)}{L_A} \equiv \frac{U(L_B)}{L_B}. \tag{21}$$

Similarly, we obtain the heat released to the low temperature entropy sink in another quantum isobaric process $C \longrightarrow D$.

$$\text{đ}Q_{CD} = F_0 \times (L_C - L_D) \tag{22}$$

The efficiency of the quantum Brayton cycle based on a single-mode radiation field can be expressed as

$$\eta = 1 - \frac{F_0(L_C - L_D)}{F_1(L_B - L_A)}, \tag{23}$$

Through a similar argument to that for a single particle in a 1D box, from Eqs. (7) and (12) we have (8) and (11) $F_1 \times L_B = U(L_B)$, $F_0 \times L_C = U(L_C)$, and (in quantum adiabatic process) the relation of internal energy

$$\frac{U(L_B)}{U(L_C)} = \frac{L_C}{L_B}, \tag{24}$$

we have

$$\frac{F_1}{F_0} = \left(\frac{L_C}{L_B} \right)^2. \tag{25}$$

Hence, from Eqs. (23) and (25) we obtain the expression of efficiency (23) of a quantum Brayton cycle based on a quantum harmonic oscillator

$$\eta = 1 - \sqrt{\frac{F_0}{F_1}} \tag{26}$$

From Eq. (11) we know that in a quantum adiabatic process, $TL = const$ or $\gamma = 2$ for single-mode radiation field. It can be seen that the efficiency of a quantum Brayton cycle obtained here (26) is the same as that of a classical Brayton cycle.

IV. QUANTUM DIESEL CYCLE

Except for the above thermodynamic cycles consisting of two pair of basic thermodynamic processes, there are some thermodynamic cycles consisting of more than two kinds of thermodynamic processes, such as Diesel cycle, which consists of two adiabatic processes, one isobaric processes and one isochcoric process [10] (see Fig. 5). In the following we will consider implementing quantum Diesel cycle in single particle in 1D box system and in single mode radiation field. First we consider the 1D box system. The input and output energy can be calculated as

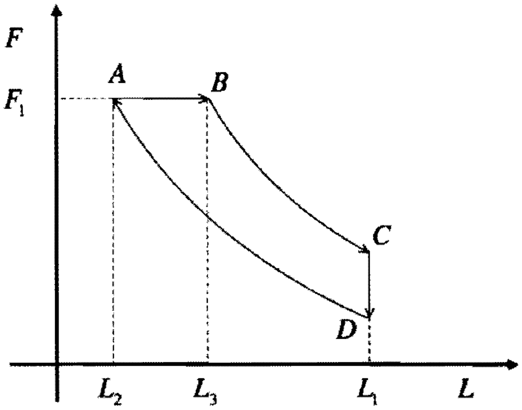

FIG. 5: Force-Displacement (Pressure-Volume) $F - L$ diagram of a quantum Diesel cycle based on a single particle in 1D box and single mode radiation field. $A \longrightarrow B$ represents an isobaric expansion process with a constant pressure F_1; $B \longrightarrow C$ represents an adiabatic expansion process with constant entropy; $C \longrightarrow D$ represents an isochoric compression process with constant volume L_1; $D \longrightarrow A$ is another adiabatic compression process.

$$\begin{aligned} Q_{in} &= C_P(T_B - T_A) \\ Q_{out} &= C_V(T_C - T_D) \end{aligned} \tag{27}$$

Thus the efficiency of the quantum Diesel cycle can be expressed in terms of specific heat and temperature

$$\eta = \frac{Q_{in} - Q_{out}}{Q_{in}} = 1 - \frac{C_V(T_C - T_D)}{C_P(T_B - T_A)}. \tag{28}$$

It is convenient to express this efficiency in terms of compression ration $r_C = \frac{V_2}{V_1}$ (see Fig. 5) and the expansion ratio $r_E = \frac{V_3}{V_1}$ (see Fig. 5). Now using the equation of state $FL = kT$ (5) and $\frac{C_P}{C_V} = \gamma = 3$ for a single particle in a box. The efficiency can be rewritten as

$$\eta = 1 - \frac{1}{3}\frac{(F_C L_C - F_D L_D)}{(F_B L_B - F_A L_A)}. \tag{29}$$

By utilizing the fact $L_C = L_D = L_1$, and $F_A = F_B = F_1$ (see Fig. 5), we further simplify the Eq. (29) to

$$\eta = 1 - \frac{1}{3}\frac{L_1(F_C - F_D)}{F_1(L_B - L_A)} = 1 - \frac{1}{3}\frac{(\frac{F_C}{F_1} - \frac{F_D}{F_1})}{(r_E - r_C)}. \tag{30}$$

Finally by making use of the adiabatic condition $FL^3 = const$ in $B \longrightarrow C$ and $D \longrightarrow A$

$$\begin{aligned} \frac{F_C}{F_1} &= \left(\frac{L_3}{L_1}\right)^3 = r_E^3, \\ \frac{F_D}{F_1} &= \left(\frac{L_2}{L_1}\right)^3 = r_C^3, \end{aligned} \tag{31}$$

the efficiency can be written as

$$\eta = 1 - \frac{1}{3}\frac{r_E^3 - r_C^3}{r_E - r_C} = 1 - \frac{1}{3}(r_E^2 + r_C^2 + r_C^2). \tag{32}$$

This efficiency for a Diesel cycle based on a single-particle in 1D box agrees with that of a classical Diesel cycle. Similarly we obtain the efficiency for single radiation field with the only change of γ from 3 to 2

$$\eta = 1 - \frac{1}{2}\frac{r_E^2 - r_C^2}{r_E - r_C} = 1 - \frac{1}{2}(r_E + r_C) \tag{33}$$

Before concluding this section, we would like to mention that we can also discuss a quantum brayton cycle and quantum Diesel cycle based on any quantum system, such as black body radiation field or a spin-1/2 in an external magnetic field with the Hamiltonian $H = \frac{1}{2}B(\sigma_z)$. As we have mentioned before, the efficiency of quantum Brayton cycle and quantum Diesel cycle is the same as their classical counter part. As long as we get the adiabatic exponent, we obtain the explicit expression of their efficiency. For a spin-1/2, we choose the inverse of the magnetic field strength as the generalized coordinate $L = \frac{1}{B}$. It can be proved that the adiabatic exponent for such a system is $\gamma = 2$. As a result, the efficiency of a Brayton cycle based on a spin-1/2 is the same as that based on a single-mode radiation field (26). The efficiency for Brayton cycle and Diesel cycle based on radiation field can be obtained straightforwardly by the adiabatic exponent. In Table II we list the working efficiency for several typical thermodynamic cycles based on different kinds of quantum working substance.

V. REMARKS AND CONCLUSIONS

In this paper, we study the quantum mechanical analogue of isobaric processes based on a microscopic definition of force, and make quantum mechanical generalization of some typical thermodynamic cycles based on quantum isobaric processes. The properties of these quantum thermodynamic processes and cycles are clarified. Through the comparison of

TABLE I: Typical classical thermodynamic processes and their quantum counterparts. Here the classical thermodynamic processes are studied based on classical ideal gas, and the quantum thermodynamic processes are studied based on the 1D infinite square potential system. We illustrate the equation of state for the four basic thermodynamic processes and we also indicate the invariant or varying observable in these processes.

	Isothermal ($T \equiv T_0$)	**Isochoric** ($V \equiv V_0$ or $L \equiv L_0$)	**Isobaric** ($P \equiv P_0$ or $F \equiv F_0$)	**Adiabatic** ($S \equiv S_0$)
Classical	$P(V)V = const;$ VRA: S, V, P; INV: T	$\frac{P(T)}{T} = const;$ VRA: S, T, P; INV: V	$\frac{V(T)}{T} = const;$ VRA: S, T, V; INV: P,	$P(T)V^3(T) = const;$ VRA: V, T P; INV: S
Quantum	$F(L)L = const;$ VRA: S, E_n, P_n; INV: T	$\frac{F(T)}{T} = const;$ VRA: S, T, P_n; INV: E_n	$\frac{L(T)}{T} = const;$ VRA: S, T, E_n, P_n;	$F(T)L^3(T) = const;$ VRA: E_n, T; INV: , P_n, S

TABLE II: Typical classical thermodynamic cycles and their quantum counterparts. Different working substance are considered here. It can be seen that both quantum thermodynamic cycles and classical thermodynamic cycles has the same efficiency up to a the adiabatic exponent γ. Adiabatic exponent for classical idea gas can be found in [20]. It can be seen that performance of the Carnot cycle is independent of the working substance, while the performance of other cycles, in general, depend on the properties of the working substance.

		Carnot (two isothermal + two adiabatic) $\eta = 1 - \frac{T_C}{T_H}$	**Otto** (two isochoric+ two adiabatic) $\eta = 1 - \left(\frac{V_0}{V_1}\right)^{\gamma-1}$	**Brayton** (two isobaric + two adiabatic) $\eta = 1 - \left(\frac{P_0}{P_1}\right)^{1-\frac{1}{\gamma}}$	**Diesel** (isochoric + isobaric + two isobaric) $\eta = 1 - \frac{1}{\gamma}\frac{\left(\frac{V_2}{V_1}\right)^{\gamma}-\left(\frac{V_3}{V_1}\right)^{\gamma}}{\left(\frac{V_2}{V_1}\right)-\left(\frac{V_3}{V_1}\right)}$
Classical	Monoatomic classical idea gas ($\gamma = \frac{5}{3}$)	$\eta = 1 - \frac{T_C}{T_H}$	$\eta = 1 - \left(\frac{V_0}{V_1}\right)^{\frac{2}{3}}$	$\eta = 1 - \left(\frac{P_0}{P_1}\right)^{\frac{2}{5}}$	$\eta = 1 - \frac{3}{5}\frac{\left(\frac{V_2}{V_1}\right)^{\frac{5}{3}}-\left(\frac{V_3}{V_1}\right)^{\frac{5}{3}}}{\left(\frac{V_2}{V_1}\right)-\left(\frac{V_3}{V_1}\right)}$
	Diatomic classical idea gas ($\gamma = \frac{7}{5}$)	$\eta = 1 - \frac{T_C}{T_H}$	$\eta = 1 - \left(\frac{V_0}{V_1}\right)^{\frac{2}{5}}$	$\eta = 1 - \left(\frac{P_0}{P_1}\right)^{\frac{2}{7}}$	$\eta = 1 - \frac{5}{7}\frac{\left(\frac{V_2}{V_1}\right)^{\frac{7}{5}}-\left(\frac{V_3}{V_1}\right)^{\frac{7}{5}}}{\left(\frac{V_2}{V_1}\right)-\left(\frac{V_3}{V_1}\right)}$
	Polyatomic classical idea gas ($\gamma = \frac{4}{3}$)	$\eta = 1 - \frac{T_C}{T_H}$	$\eta = 1 - \left(\frac{V_0}{V_1}\right)^{\frac{1}{3}}$	$\eta = 1 - \left(\frac{P_0}{P_1}\right)^{\frac{1}{4}}$	$\eta = 1 - \frac{3}{4}\frac{\left(\frac{V_2}{V_1}\right)^{\frac{4}{3}}-\left(\frac{V_3}{V_1}\right)^{\frac{4}{3}}}{\left(\frac{V_2}{V_1}\right)-\left(\frac{V_3}{V_1}\right)}$
Quantum	Single particle in 1D box ($\gamma = 3$)	$\eta = 1 - \frac{T_C}{T_H}$	$\eta = 1 - \left(\frac{L_0}{L_1}\right)^{2}$	$\eta = 1 - \left(\frac{F_0}{F_1}\right)^{\frac{2}{3}}$	$\eta = 1 - \frac{1}{3}\frac{\left(\frac{L_2}{L_1}\right)^{3}-\left(\frac{L_3}{l_1}\right)^{3}}{\left(\frac{L_2}{L_1}\right)-\left(\frac{L_3}{L_1}\right)}$
	Single particle in 2D box ($\gamma = 2$)	$\eta = 1 - \frac{T_C}{T_H}$	$\eta = 1 - \left(\frac{S_0}{S_1}\right)^{1}$	$\eta = 1 - \left(\frac{P_0}{P_1}\right)^{\frac{1}{2}}$	$\eta = 1 - \frac{1}{2}\frac{\left(\frac{S_2}{S_1}\right)^{2}-\left(\frac{S_3}{S_1}\right)^{2}}{\left(\frac{S_2}{S_1}\right)-\left(\frac{S_3}{S_1}\right)}$
	Single particle in 3D box ($\gamma = \frac{5}{3}$)	$\eta = 1 - \frac{T_C}{T_H}$	$\eta = 1 - \left(\frac{V_0}{V_1}\right)^{\frac{2}{3}}$	$\eta = 1 - \left(\frac{P_0}{P_1}\right)^{\frac{2}{5}}$	$\eta = 1 - \frac{3}{5}\frac{\left(\frac{V_2}{V_1}\right)^{\frac{5}{3}}-\left(\frac{V_3}{V_1}\right)^{\frac{5}{3}}}{\left(\frac{V_2}{V_1}\right)-\left(\frac{V_3}{V_1}\right)}$
	Single mode photon field ($\gamma = 2$)	$\eta = 1 - \frac{T_C}{T_H}$	$\eta = 1 - \left(\frac{L_0}{L_1}\right)^{1}$	$\eta = 1 - \left(\frac{F_0}{F_1}\right)^{\frac{1}{2}}$	$\eta = 1 - \frac{1}{2}\frac{\left(\frac{L_2}{L_1}\right)^{2}-\left(\frac{L_3}{l_1}\right)^{2}}{\left(\frac{L_2}{L_1}\right)-\left(\frac{L_3}{L_1}\right)}$
	Black body radiation field ($\gamma = \frac{4}{3}$)	$\eta = 1 - \frac{T_C}{T_H}$	$\eta = 1 - \left(\frac{V_0}{V_1}\right)^{\frac{1}{3}}$	$\eta = 1 - \left(\frac{P_0}{P_1}\right)^{\frac{1}{4}}$	$\eta = 1 - \frac{3}{4}\frac{\left(\frac{V_2}{V_1}\right)^{\frac{4}{3}}-\left(\frac{V_3}{V_1}\right)^{\frac{4}{3}}}{\left(\frac{V_2}{V_1}\right)-\left(\frac{V_3}{V_1}\right)}$
	1D harmonic oscillator ($\gamma = 2$)	$\eta = 1 - \frac{T_C}{T_H}$	$\eta = 1 - \left(\frac{L_0}{L_1}\right)^{1}$	$\eta = 1 - \left(\frac{F_0}{F_1}\right)^{\frac{1}{2}}$	$\eta = 1 - \frac{1}{2}\frac{\left(\frac{L_2}{L_1}\right)^{2}-\left(\frac{L_3}{l_1}\right)^{2}}{\left(\frac{L_2}{L_1}\right)-\left(\frac{L_3}{L_1}\right)}$
	2D harmonic oscillator ($\gamma = \frac{3}{2}$)	$\eta = 1 - \frac{T_C}{T_H}$	$\eta = 1 - \left(\frac{S_0}{S_1}\right)^{\frac{1}{2}}$	$\eta = 1 - \left(\frac{P_0}{P_1}\right)^{\frac{1}{3}}$	$\eta = 1 - \frac{2}{3}\frac{\left(\frac{S_2}{S_1}\right)^{\frac{3}{2}}-\left(\frac{S_3}{S_1}\right)^{\frac{3}{2}}}{\left(\frac{S_2}{S_1}\right)-\left(\frac{S_3}{S_1}\right)}$
	3D harmonic oscillator ($\gamma = \frac{4}{3}$)	$\eta = 1 - \frac{T_C}{T_H}$	$\eta = 1 - \left(\frac{V_0}{V_1}\right)^{\frac{1}{3}}$	$\eta = 1 - \left(\frac{P_0}{P_1}\right)^{\frac{1}{4}}$	$\eta = 1 - \frac{3}{4}\frac{\left(\frac{V_2}{V_1}\right)^{\frac{4}{3}}-\left(\frac{V_3}{V_1}\right)^{\frac{4}{3}}}{\left(\frac{V_2}{V_1}\right)-\left(\frac{V_3}{V_1}\right)}$
	spin-1/2 (2-level system) ($\gamma = 2$)	$\eta = 1 - \frac{T_C}{T_H}$	$\eta = 1 - \left(\frac{L_0}{L_1}\right)^{1}$	$\eta = 1 - \left(\frac{F_0}{F_1}\right)^{\frac{1}{2}}$	$\eta = 1 - \frac{1}{2}\frac{\left(\frac{L_2}{L_1}\right)^{2}-\left(\frac{L_3}{l_1}\right)^{2}}{\left(\frac{L_2}{L_1}\right)-\left(\frac{L_3}{L_1}\right)}$

quantum thermodynamics with classical thermodynamics, we find that the properties of these quantum thermodynamic processes and cycles agrees well with those thermodynamic processes and cycles based on classical ideal gas. We give the microscopic (quantum mechanical) explanation of Szilard-Zurek single molecule engine (operating in a different thermodynamic cycle).

Before concluding this work, we would like to mention that in our current work we focus on the quantum single-particle system, and its related quantum mechanical generalization of heat, work, pressure. We also notice some work about quantum heat engine with quantum many body system as the working substance [18]. For real quantum many body system, e.g., ideal bosonic gas or ideal fermionic gas, the mechanic observable, such as heat work, pressure, are well defined and their equation of state as well as their expression of internal energy [19] deviate from that of the classical ideal gas. As a result, the quantum thermodynamic cycles based on the quantum many-body system deviate from that of classical ideal gas due to quantum degeneracy. Our current discussion focus on ideal thermodynamic cycle only. That is, we consider only quasi-static process. Similar to the discussion about finite-power Carnot engine [21], Dinite-power analysis of Brayton cycle and Diesel cycle will be given later

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