

Quantum coherence in a quantum heat engine

Yun-Hao Shi^{1,2,3} , Hai-Long Shi^{4,5}, Xiao-Hui Wang^{1,7},
Ming-Liang Hu⁸ , Si-Yuan Liu^{2,6,7}, Wen-Li Yang^{1,6,7}
and Heng Fan^{2,3,9}

¹ School of Physics, Northwest University, Xi'an 710127, People's Republic of China

² Institute of Physics, Chinese Academy of Sciences, Beijing 100190, People's Republic of China

³ School of Physical Sciences & CAS Center for Excellence in Topological Quantum Computation, UCAS, Beijing 100190, People's Republic of China

⁴ State Key Laboratory of Magnetic Resonance and Atomic and Molecular Physics, Wuhan Institute of Physics and Mathematics, Chinese Academy of Sciences, Wuhan 430071, People's Republic of China

⁵ University of Chinese Academy of Sciences, Beijing 100049, People's Republic of China

⁶ Institute of Modern Physics, Northwest University, Xi'an 710127, People's Republic of China

⁷ Shaanxi Key Laboratory for Theoretical Physics Frontiers, Xi'an 710127, People's Republic of China

⁸ School of Science, Xi'an University of Posts and Telecommunications, Xi'an 710121, People's Republic of China

⁹ Songshan Lake Materials Laboratory, Dongguan 523808, People's Republic of China

E-mail: xhwang@nwu.edu.cn (Xiao-Hui Wang) and hfan@iphy.ac.cn (Heng Fan)

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Abstract

We identify that quantum coherence is a valuable resource in the quantum heat engine, which is designed in a quantum thermodynamic cycle assisted by a quantum Maxwell's demon. This demon is in a superposed state. The quantum work and heat are redefined as the sum of coherent and incoherent parts in the energy representation. The total quantum work and the corresponding efficiency of the heat engine can be enhanced due to the coherence consumption of the demon. In addition, we discuss an universal information heat engine driven by quantum coherence. The extractable work of this heat engine is limited by the quantum coherence, even if it has no classical thermodynamic cost. This resource-driven viewpoint provides a direct and effective way to clarify the thermodynamic processes where the coherent superposition of states cannot be ignored.

Keywords: quantum coherence, quantum heat engine,
quantum thermodynamics

(Some figures may appear in colour only in the online journal)

1. Introduction

Quantum information theory [1, 2] plays a crucial role in thermodynamics [3–12]. Specifically, the rigorous frameworks for the quantification of quantum coherence [13–16] and quantum correlations, such as entanglement [17] and discord [18], bring new insights into our understanding about quantum effects in thermodynamics. Those new concepts created from quantum information motivate us to reconsider the physical origin of thermodynamic notions such as work, heat, efficiency of heat engine etc.

On the other hand, remarkable progress of quantum thermodynamics began with the fundamental relations in non-equilibrium statistical mechanics known as the Jarzynski equality [19, 20] or fluctuation theorems [21–24], which lead to the second law of thermodynamics as a corollary. The Maxwell’s demon [28], as an intermediary, bridges information and thermodynamics [30], such as Landauer’s principle [36, 37] and generalized second laws [24–27]. All of these support the view that information is a sort of physical existence, contributing to the adaptation of thermodynamics to quantum physics. Existing approaches to quantum thermodynamics are mainly based on operator formalisms [6, 21], which provides a general framework for the thermodynamics of information. Another approach to quantum thermodynamics is path integral formalism [39] based on two-point measurement scheme [20, 40]. This approach provides an effective way to calculate quantum work by utilizing various path integral techniques. However, it is still difficult to figure out where information plays an important role and what kind of information is useful in a specific case, since both classical information and quantum information facilitate thermodynamic processes. It is interesting to explore such problems [3, 38].

As is known, quantum coherence describes the departure of quantum mechanics from the classical realm. It is a natural idea to interpret fundamental thermodynamic notions of quantum system by identifying the behaviour of quantum coherence and combining it with the same basic problem—Maxwell’s demon [28]. Maxwell’s demon has been a fundamental research question and topical issues for statistical mechanics and thermodynamics. Here we consider the object of quantum Maxwell’s demon (QMD) in a quantum heat engine. This type of heat engine assisted by one quantum system has been extensively studied [30–32]. The other two types of engines are based on the parametric oscillator [33, 34] and the invasive quantum measurement without feedback control [35], respectively. In this paper, we are more concerned about that when the demon is in a superposed state, how its quantum coherence disturbs the whole thermodynamic cycle of the heat engine. The ultimate goal is to explore the behaviour and role of quantum coherence in quantum thermodynamics.

This paper is organized as follows. Firstly, we discuss briefly the resource-theoretic framework of quantum coherence and introduce the QMD with coherence as the control unit in a quantum heat engine. Subsequently, the whole thermodynamic cycle of the heat engine assisted by QMD is studied, and the effects of quantum coherence on the fundamental thermodynamic notions are investigated. In addition, we reinvestigate the information heat engine (IHE) assisted by one memory with coherence, as an universal heat engine driven by quantum coherence. Meanwhile, we calculate the maximum work extractable with the coherence consumption. Finally, more general thermodynamics involving quantum coherence is considered.

2. Quantum coherence and quantum Maxwell's demon

The rigorous framework for quantifying quantum coherence was first introduced by Baumgratz *et al* who proposed four criteria for coherence measures [13]. One well-defined measure is the relative entropy of coherence, which takes the form [13–16]

$$C_r(\rho) := \min_{\sigma \in \mathcal{I}} S(\rho||\sigma) = S(\rho_{\text{diag}}) - S(\rho), \quad (1)$$

where \mathcal{I} denotes the set of incoherent states, $S(\rho) = -\text{Tr}(\rho \ln \rho)$ is the von Neumann entropy [1] and ρ_{diag} is the state obtained from ρ by deleting all the off diagonal elements. In the reference basis $|i\rangle$, ρ_{diag} can be expressed as $\sum_i \langle i|\rho|i\rangle |i\rangle\langle i|$. This entropic measure of coherence has a clear physical interpretation and many applications [15]. For instance, quantum coherence can enhance the success probability in Grover search quantum algorithm [45]. In [46], physical situations have been considered where the resource theories of coherence and thermodynamics play competing roles, especially the creation of quantum coherence comes at a cost of energy. Therefore, coherence can be viewed as a potential quantum resource in quantum physical processes. Exploring more applications of quantum coherence is of wide interests.

To investigate quantum coherence effect in quantum thermodynamics, we introduce a basic problem of statistical mechanics—the paradox of Maxwell's demon [28], whose role of the information was firstly studied by Szilard [29, 30]. A classical Maxwell's demon (CMD) can be described as an incoherent state, whereas a QMD with off-diagonal elements is in a coherent state, namely

$$\rho_D = p_g |g\rangle\langle g| + p_e |e\rangle\langle e| + F |g\rangle\langle e| + F^* |e\rangle\langle g|, \quad (2)$$

where p_g and $p_e = 1 - p_g$ are the probability distributions in the ground state $|g\rangle$ and excited state $|e\rangle$, respectively. QMD can be viewed as an arbitrary single-qubit system expressed in the Bloch sphere (see figure 1). The off-diagonal elements F and F^* are introduced to embody the quantum coherence. The QMD and its related second law-like equalities (inequalities) have already been experimentally verified by using various systems in recent years [50–56].

According to equations (1) and (2), the coherence of QMD can be written as

$$C_r(\rho_D) = H(p_g) - H(\lambda_+), \quad (3)$$

where $H(x) = H(1-x) = -x \ln x - (1-x) \ln(1-x)$ is the Shannon entropy function [1] and $\lambda_{\pm} = \frac{1}{2}(1 \pm \sqrt{(p_g - p_e)^2 + 4|F|^2})$ are the eigenvalues of ρ_D . If we set ρ_D as the initial state of QMD in the heat engine ρ_D^i , the initial coherence is exactly in the form of equation (3).

In what follows, we will focus on the analysis of the whole quantum thermodynamic cycle assisted by QMD based on quantum Szilard engine (QSE) [43, 49] and reveal the behavior and role of quantum coherence.

3. Quantum Maxwell's demon with coherence assisted quantum thermodynamic cycle

As a carrier of coherence, QMD is typically designed to drive a QSE [43, 44], which consists of a closed box with definite size L and one system S (such as a single molecule). The demon in our thermodynamic cycle is in contact with a lower temperature heat bath while the system's bath is at a higher temperature. Although the system is in equilibrium, the QMD is in a nonequilibrium state, as a unit to control expansion. In the cycle, the quantum coherence of the demon is consumed continuously, contributing to the extra work.

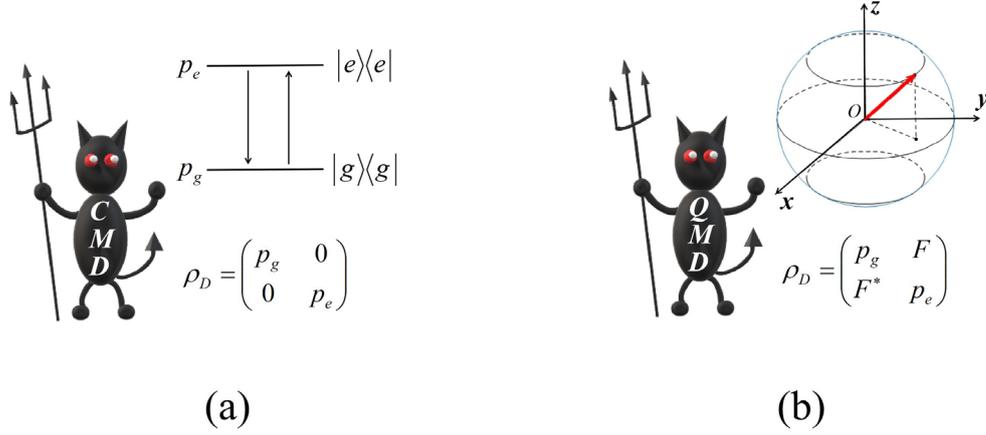


Figure 1. Classical Maxwell's demon (CMD) versus quantum Maxwell's demon (QMD). (a) CMD can be considered as a classical mixture of two definite eigenstates $|g\rangle$ and $|e\rangle$, while QMD with coherence should be preferred to a qubit described in the Bloch sphere, as shown in (b). Here, $p_g = (1 + z)/2$, $p_e = (1 - z)/2$, $F = (x - iy)/2$ and $F^* = (x + iy)/2$ are the classical probability distribution of ground state and excited state, and its off-diagonal elements, respectively. Note that $x^2 + y^2 + z^2 \leq 1$, thus $|F|^2 \leq p_g p_e$, where the equality is achieved if it is a pure quantum state.

The whole thermodynamic cycle is briefly shown in figure 2, which is split into five stages: (i) Initial state, (ii) Insertion, (iii) Measurement, (iv) Expansion, and (v) Removal. At the stage of insertion, a wall is isothermally inserted at location l . We denote P_L as the quantum probability of the system S on the left after insertion, then $P_R = 1 - P_L$ is the probability of S on the right. What the QMD should do are performing a global measurement both on the system S and itself (the controlled-NOT operation [47–49]), and then controlling the expansion of S . When the wall is removed and this thermodynamic cycle is completed, S returns to its initial state of equilibrium. In the presence of quantum coherence, it is insufficient to know its diagonal part. Instead, we describe the evolution of the whole system in terms of the full density matrix.

Stage (i): Initial state.—Initially, the system S , prepared in a closed box with size L , contacts with the reservoir at temperature $T = (k_B \beta)^{-1}$ so that it is in equilibrium. With the initial Hamiltonian $H_S = \sum_n E_n(L) |\psi_n(L)\rangle \langle \psi_n(L)|$, the density matrix of the initial state of the total system can be written as a product state

$$\begin{aligned} \rho^i &= \rho_S^i \otimes \rho_D^i \\ &= \sum_n \frac{e^{-\beta E_n(L)}}{Z(L)} |\psi_n(L)\rangle \langle \psi_n(L)| \otimes \rho_D^i, \end{aligned} \quad (4)$$

where $Z(L) = \sum_n e^{-\beta E_n(L)}$, $E_n(L)$ and $|\psi_n(L)\rangle$ are the partition function, n th eigenenergy and eigenstate of the system S in this box with size L . Here, the initial density matrix of QMD, namely ρ_D^i takes the form of equation (2).

The system S will always be in the isothermal process with the reservoir, leading to its thermalization so that all the coherence among energy levels vanishes [43]. Even so, it is necessary to describe the dynamics of the total system in terms of the full density matrix, because our QMD with off-diagonal elements is still coherent at another temperature $T_D = (k_B \beta_D)^{-1}$.

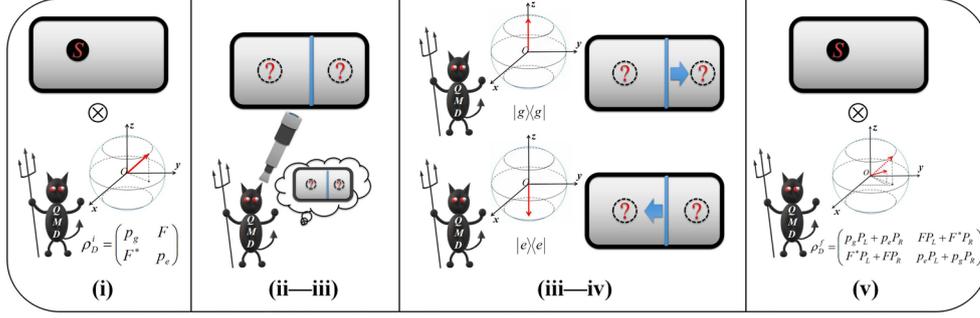


Figure 2. Schematic diagram of the quantum thermodynamic cycle assisted by quantum Maxwell’s demon (QMD). (i) A system S is prepared in a closed box with size L while QMD with coherence is isolated from the box. (ii)–(iii) A wall, depicted by a vertical blue bar, is isothermally inserted at location l . And the measurement is performed later to register the information of the system S into QMD’s memory. (iii)–(iv) According to the state of the quantum memory, the wall controlled by QMD undergoes a reversible and isothermal expansion until it reaches equilibrium. (v) To complete this thermodynamic cycle, the wall is removed isothermally. At the moment, the state of QMD is overwhelmingly different from the initial state and its coherence has been consumed.

Here we emphasize that our discussion does not depend on a specific model. For instance, the box does not have to be an infinite potential well model, i.e. the eigenenergies and eigenfunctions of the system S are $E_n(L) = \hbar^2 \pi^2 n^2 / (2mL^2)$ and $\langle x | \psi_n(L) \rangle = \sqrt{2/L} \sin(\pi n x / L)$, where the quantum number n ranges from 1 to ∞ .

Stage (ii): Insertion.—After preparing initial state, a wall is then isothermally inserted at a certain position l . In the classical situation, the position of the system S is definite, so either it is on the left side or stay on the right side, while in the quantum case the system is simultaneously on both sides of the wall, until its location is determined by the measurement of the observer. Therefore, when the wall insertion is completed, the total density matrix can be expressed as a mixture, namely

$$\rho^{\text{ins}} = [P_L \rho^L(l) + P_R \rho^R(L-l)] \otimes \rho_D^i, \quad (5)$$

where $\rho^L(l) = \sum_n \frac{e^{-\beta E_n(l)}}{Z(l)} |\psi_n^L(l)\rangle \langle \psi_n^L(l)|$ and $\rho^R(L-l) = \sum_n \frac{e^{-\beta E_n(L-l)}}{Z(L-l)} |\psi_n^R(L-l)\rangle \langle \psi_n^R(L-l)|$ are the independent densities of S on the left and right sides, $P_L = Z(l) / [Z(l) + Z(L-l)]$ and $P_R = 1 - P_L$ are the corresponding quantum probabilities, which differ from the classical probabilities $P_L^{\text{classical}} = l/L$ and $P_R^{\text{classical}} = (L-l)/L$ [49]. In this stage, QMD is still out of work, which is the same as CMD. And because the system S has no coherence, thus the results (work, heat, etc) in this stage only relate with diagonal part of S , as in the case of no coherence in [43].

Stage (iii): Measurement.—Now the demon will perform a global measurement, which can be described by the controlled-NOT operation [48, 49], namely

$$U = \sum_n [|\psi_n^L(l)\rangle \langle \psi_n^L(l)| \otimes (|g\rangle\langle g| + |e\rangle\langle e|) + |\psi_n^R(L-l)\rangle \langle \psi_n^R(L-l)| \otimes (|e\rangle\langle g| + |g\rangle\langle e|)]. \quad (6)$$

It is easy to verify that U is a unitary operator, which is different from the positive operator valued measure (POVM) in previous discussions [58–60]. Here, the physical process

corresponding to U is that the demon will keep the original state if the system S with n levels is on the left side, while the demon flips its state when S is on the right. After this operation, the total density matrix is given by

$$\begin{aligned}\rho^{\text{mea}} &= U\rho^{\text{ins}}U^\dagger \\ &= P_L\rho^L(l) \otimes (p_g|g\rangle\langle g| + p_e|e\rangle\langle e| + F|g\rangle\langle e| + F^*|e\rangle\langle g|) \\ &\quad + P_R\rho^R(L-l) \otimes (p_e|g\rangle\langle g| + p_g|e\rangle\langle e| + F^*|g\rangle\langle e| + F|e\rangle\langle g|) \\ &= [p_gP_L\rho^L(l) + p_eP_R\rho^R(L-l)] \otimes |g\rangle\langle g| + [p_eP_L\rho^L(l) + p_gP_R\rho^R(L-l)] \otimes |e\rangle\langle e| \\ &\quad + [FP_L\rho^L(l) + F^*P_R\rho^R(L-l)] \otimes |g\rangle\langle e| + [F^*P_L\rho^L(l) + FP_R\rho^R(L-l)] \otimes |e\rangle\langle g|,\end{aligned}\tag{7}$$

which means QMD is now correlated with the system S , contributing to the work to the outside.

Compared with CMD, QMD seem to be ‘blurry-eyed’, so that it cannot exactly distinguish which side the system S stays on. In the limits of $F \rightarrow 0$ and $T_D \rightarrow 0$, $\rho^{\text{mea}} \rightarrow P_L\rho^L(l) \otimes |g\rangle\langle g| + P_R\rho^R(L-l) \otimes |e\rangle\langle e|$, which implies that QMD is ‘cured’, i.e. its ground state $|g\rangle$ corresponds to the system S on the left and vice versa, as the case of CMD.

For registering the information of the system S into QMD’s memory, the outside agent have to do work on the total system in this process, leading to the change of the total internal energy. The mean value of this work, namely $\langle W_{\text{mea}} \rangle = \text{Tr}[(H_S + H_D)(\rho^{\text{mea}} - \rho^{\text{ins}})] = P_R(p_g - p_e)\Delta$, has nothing to do with the off-diagonal elements, because the flip of off-diagonal part makes no contribution to the change of internal energy. However, the off-diagonal part has affected the total density matrix, giving rise to a more complex form about entropy and heat as the following discussions. Here, H_S and H_D are the Hamiltonian of the system and the demon, respectively. We assume that the demon is a two-level system so that $H_D = E_g|g\rangle\langle g| + E_e|e\rangle\langle e|$ and $\Delta = E_e - E_g$.

Stage (iv): Expansion.—In this stage, the expansion of the system S is slowly enough to ensure the process reversible and isothermal, which is controlled by QMD according to its memory. The wall will be allowed to move to the right side at a final position l_g if QMD is in the ground state and move to the right side at a final position l_e if the demon is in the excited state (see intuitively in figures 2(iii)–(iv)). In accordance with the above analysis, the evolution operator of the controlled expansion can be mathematically constructed as

$$\begin{aligned}O_{\text{exp}} &= \sum_n \left\{ \left[\sqrt{\frac{P_n(l_g)}{P_n(l)}} |\psi_n^L(l_g)\rangle\langle\psi_n^L(l)| + \sqrt{\frac{P_n(L-l_g)}{P_n(L-l)}} |\psi_n^R(L-l_g)\rangle\langle\psi_n^R(L-l)| \right] \otimes |g\rangle\langle g| \right. \\ &\quad \left. + \left[\sqrt{\frac{P_n(l_e)}{P_n(l)}} |\psi_n^L(l_e)\rangle\langle\psi_n^L(l)| + \sqrt{\frac{P_n(L-l_e)}{P_n(L-l)}} |\psi_n^R(L-l_e)\rangle\langle\psi_n^R(L-l)| \right] \otimes |e\rangle\langle e| \right\},\end{aligned}\tag{8}$$

where $P_n(x) = \frac{e^{-\beta E_n(x)}}{Z(x)}$. We thus obtain the total density matrix after expansion:

$$\begin{aligned}\rho^{\text{exp}} &= O_{\text{exp}}\rho^{\text{mea}}O_{\text{exp}}^\dagger \\ &= [p_gP_L\rho^L(l_g) + p_eP_R\rho^R(L-l_g)] \otimes |g\rangle\langle g| + [p_eP_L\rho^L(l_e) + p_gP_R\rho^R(L-l_e)] \otimes |e\rangle\langle e| \\ &\quad + [FP_L\rho_{l_g,l_e}^L + F^*P_R\rho_{l_g,l_e}^R] \otimes |g\rangle\langle e| + [F^*P_L\rho_{l_e,l_g}^L + FP_R\rho_{l_e,l_g}^R] \otimes |e\rangle\langle g|,\end{aligned}\tag{9}$$

where $\rho^L(l_g) = \sum_n P_n(l_g) |\psi_n^L(l_g)\rangle\langle\psi_n^L(l_g)|$ and $\rho^R(l_e) = \sum_n P_n(l_e) |\psi_n^R(l_e)\rangle\langle\psi_n^R(l_e)|$ are the post-expansion densities controlled by the diagonal parts $|g\rangle\langle g|$ and $|e\rangle\langle e|$, respectively. Similarly, the items $\rho_{l_g,l_e}^L = \sum_n \sqrt{P_n(l_g)P_n(l_e)} |\psi_n^L(l_g)\rangle\langle\psi_n^L(l_e)|$ and $\rho_{l_g,l_e}^R = \sum_n \sqrt{P_n(L-l_g)P_n(L-l_e)} |\psi_n^R(L-l_g)\rangle\langle\psi_n^R(L-l_e)|$ in equation (9) can be viewed as the post-expansion densities controlled

by the off-diagonal part $|g\rangle\langle e|$, whereas $\rho_{l_e, l_g}^L = \sum_n \sqrt{P_n(l_e)P_n(l_g)}|\psi_n^L(l_e)\rangle\langle\psi_n^L(l_g)|$ and $\rho_{l_e, l_g}^R = \sum_n \sqrt{P_n(L-l_e)P_n(L-l_g)}|\psi_n^R(L-l_e)\rangle\langle\psi_n^R(L-l_g)|$ are controlled by $|e\rangle\langle g|$.

In classical physics, the system must be on one side of the wall with another side empty after insertion, thus the wall is doomed to be moved to an end boundary of the box due to expansion. In contrast, quantum system can be simultaneously on both sides of the wall, thus the equilibrium position is somewhere in the box rather than the boundary. The condition of equilibrium, in mechanics, is that the wall has equal and opposite forces on the two sides, i.e. $F_{\text{eq}}^L = F_{\text{eq}}^R$.

Stage (v): Removal.—For purpose of the thermodynamic cycle, the system S must be reset to its own initial state, i.e. $\rho_S^i = \sum_n \frac{e^{-\beta E_n(L)}}{Z(L)}|\psi_n(L)\rangle\langle\psi_n(L)|$. The corresponding physical process is the wall inserted on the stage (ii) will be removed and all the ensembles of the system S will evolve into ρ_S^i , namely

$$\rho^{\text{rem}} = \sum_n \frac{e^{-\beta E_n(L)}}{Z(L)}|\psi_n(L)\rangle\langle\psi_n(L)| \otimes \rho_D^f \quad (10)$$

where

$$\rho_D^f = [(p_g P_L + p_e P_R)|g\rangle\langle g| + (p_e P_L + p_g P_R)|e\rangle\langle e| + (F P_L + F^* P_R)|g\rangle\langle e| + (F^* P_L + F P_R)|e\rangle\langle g|]. \quad (11)$$

In analogy with equation (8), we can also construct an operation O_{rem} to obtain equation (10), i.e. $\rho^{\text{rem}} = O_{\text{rem}}\rho^{\text{exp}}O_{\text{rem}}^\dagger$ with

$$O_{\text{rem}} = \sum_n \left\{ \left[\sqrt{\frac{P_n(L)}{P_n(l_g)}}|\psi_n(L)\rangle\langle\psi_n^L(l_g)| + \sqrt{\frac{P_n(L)}{P_n(L-l_g)}}|\psi_n(L)\rangle\langle\psi_n^R(L-l_g)| \right] \otimes |g\rangle\langle g| + \left[\sqrt{\frac{P_n(L)}{P_n(l_e)}}|\psi_n(L)\rangle\langle\psi_n^L(l_e)| + \sqrt{\frac{P_n(L)}{P_n(L-l_e)}}|\psi_n(L)\rangle\langle\psi_n^R(L-l_e)| \right] \otimes |e\rangle\langle e| \right\}. \quad (12)$$

Here we emphasize that the system S has been reset to thermal equilibrium state with no coherence, but this is not the requirement for QMD. The state of QMD remains coherent, but obviously it's much less coherent than it was at the beginning. This implies that the coherence consumption may be a direct linkage to work and heat in the whole thermodynamic cycle, as discussed below.

4. Enhancing efficiency via coherence consumption of quantum Maxwell's demon

What we have talked above is the evolution of state of the total system. Because of the coherence, it is insufficient to know its diagonal part. Instead, we describe the evolution of our system in terms of the full density matrix, which is split into five, namely Stage (i)–(v). As seen in the follows, this approach is in support of studying what we are more concerned, i.e. whether the efficiency of this quantum thermodynamics cycle could be enhanced due to the coherent QMD.

First of all, let us calculate the change of total internal energy $\langle\Delta E_{\text{tot}}\rangle$ by taking ρ^{rem} as the final density ρ^f at the end of this thermodynamics cycle. Focusing on the initial and final states, we can obtain

$$\langle \Delta E_{\text{tot}} \rangle = \langle E_f \rangle - \langle E_i \rangle = \text{Tr}[(\rho^f - \rho^i)(H_S + H_D)] = P_R(p_g - p_e)\Delta, \quad (13)$$

where $H_D = E_g|g\rangle\langle g| + E_e|e\rangle\langle e|$ is the demon's Hamiltonian and $\Delta = E_e - E_g$ is the gap of the two levels of QMD. Here, the result is independent of H_S , namely the form of the Hamiltonian of the system S is inessential during the cycle. Note that $\langle \Delta E_{\text{tot}} \rangle = \langle W_{\text{mea}} \rangle$, i.e. the change of total internal energy merely results from the work done by the outside agent during measurement, as what mentioned before. Equation (13) also confirms the fact that the change of internal energy does not involve the off-diagonal part at all.

Another important thermodynamic quantity is the total heat $\langle Q_{\text{tot}} \rangle$ absorbed from the outside, which is associated with the total entropy change due to the reversibility, namely

$$\begin{aligned} \langle Q_{\text{tot}} \rangle &= k_B T [S(\rho^f) - S(\rho^i)] \\ &= k_B T \left[S \left(\sum_n \frac{e^{-\beta E_n(L)}}{Z(L)} |\psi_n(L)\rangle\langle\psi_n(L)| \otimes \rho_D^f \right) - S \left(\sum_n \frac{e^{-\beta E_n(L)}}{Z(L)} |\psi_n(L)\rangle\langle\psi_n(L)| \otimes \rho_D^i \right) \right] \\ &= k_B T [S(\rho_D^f) - S(\rho_D^i)] \\ &= T(\Delta S_c + k_B \Delta C_r), \end{aligned} \quad (14)$$

where the second to the last line follows from the subadditivity equality for von Neumann entropy [1] and the last line follows from the definition of the coherence consumption $\Delta C_r := C_r(\rho^i) - C_r(\rho^f) = C_r(\rho_D^i) - C_r(\rho_D^f)$, and $\Delta S_c := k_B \Delta S_{\text{diag}} = k_B [S(\rho_{\text{diag}}^f) - S(\rho_{\text{diag}}^i)] = k_B [S(\rho_{D\text{diag}}^f) - S(\rho_{D\text{diag}}^i)]$. According to what we discussed above, the initial density matrix and the final density matrix are expressed as

$$\rho_D^i = \begin{pmatrix} p_g & F \\ F^* & p_e \end{pmatrix} \quad (15)$$

and

$$\rho_D^f = \begin{pmatrix} p_g P_L + p_e P_R & F P_L + F^* P_R \\ F^* P_L + F P_R & p_g P_R + p_e P_L \end{pmatrix}, \quad (16)$$

respectively. Hence, one can obtain the change of classical entropy

$$\begin{aligned} \Delta S_c &= k_B [S(\rho_{D\text{diag}}^f) - S(\rho_{D\text{diag}}^i)] \\ &= k_B [p_g \ln p_g + p_e \ln p_e - (p_g P_L + p_e P_R) \ln (p_g P_L + p_e P_R) - (p_e P_L + p_g P_R) \ln (p_e P_L + p_g P_R)] \end{aligned} \quad (17)$$

and the coherence consumption

$$\Delta C_r = C_r(\rho_D^i) - C_r(\rho_D^f) = S(\rho_D^f) - S(\rho_D^i) - \Delta S_c / k_B. \quad (18)$$

Note that in the classical process, the heat without coherence can be denoted as $\langle Q_{\text{incoh}} \rangle = T \Delta S_{\text{diag}}$, which just depends on the diagonal part. In general, we specify

$$\langle Q_{\text{tot}} \rangle = \langle Q_{\text{incoh}} \rangle + \langle Q_{\text{coh}} \rangle \quad (19)$$

as the total heat absorbed from the outside, where the coherent item $\langle Q_{\text{coh}} \rangle = k_B T \Delta C_r$ is proportional to the coherence consumption ΔC_r .

Then if we still believe that the first law holds, i.e. $\langle \Delta E_{\text{tot}} \rangle = \langle Q_{\text{tot}} \rangle - \langle W_{\text{tot}} \rangle$, the total work $\langle W_{\text{tot}} \rangle$ done by the system to the outside will be expressed as

$$\langle W_{\text{tot}} \rangle = T(\Delta S_c + k_B \Delta C_r) - P_R(p_g - p_e)\Delta. \quad (20)$$

An alternative derivation of this result can be constructed by using $\langle W_{\text{tot}} \rangle = \Delta F$ with the standard free energy $F(\rho) = \text{Tr}(H\rho) - TS(\rho)$ [3, 9], which is a special case of the general free energy $F_\alpha(\rho) = F_{\text{eq}} + TD_\alpha(\rho||\rho_{\text{eq}})$ based on quantum Renyi entropies $D_\alpha(\rho||\rho_{\text{eq}})$ when $\alpha \rightarrow 1$ [10–12].

In analogy to equation (19), the total work can be split into

$$\langle W_{\text{tot}} \rangle = \langle W_{\text{incoh}} \rangle + \langle W_{\text{coh}} \rangle, \quad (21)$$

where the incoherent work is $\langle W_{\text{incoh}} \rangle = \langle Q_{\text{incoh}} \rangle + \langle \Delta E_{\text{tot}} \rangle = T\Delta S_c - P_R(p_g - p_e)\Delta$ and $\langle W_{\text{coh}} \rangle = \langle Q_{\text{coh}} \rangle = k_B T \Delta C_r$ represents the coherent part.

Now turn to the crucial efficiency, which is defined as dividing the total work done by the system to the outside by total heat absorbed from the outside, namely

$$\eta = \frac{\langle W_{\text{tot}} \rangle}{\langle Q_{\text{tot}} \rangle} = 1 - \frac{P_R(p_g - p_e)\Delta}{T(\Delta S_c + k_B \Delta C_r)}. \quad (22)$$

Note that the coherence consumption appears in the denominator of the minuend, which implies the efficiency can be improved due to the coherence consumption of QMD. The more coherence consumed, the higher efficiency we can obtain. If there is no coherence being consumed, i.e. $\Delta C_r = 0$, it will be limited by Carnot efficiency

$$\begin{aligned} \eta_{\text{max}} &\geq \max \left\{ 1 - \frac{P_R(p_g - p_e)\Delta}{k_B T \Delta S_c} \right\} \\ &= \lim_{P_R \rightarrow 0} \left\{ 1 - \frac{(k_B T)^{-1} P_R (p_g - p_e) \Delta}{p_g \ln p_g + p_e \ln p_e - (p_g P_L + p_e P_R) \ln (p_g P_L + p_e P_R) - (p_e P_L + p_g P_R) \ln (p_e P_L + p_g P_R)} \right\} \\ &= \lim_{P_R \rightarrow 0} \left\{ 1 - \frac{(k_B T)^{-1} P_R (p_g - p_e) \Delta}{p_g \ln p_g + p_e \ln p_e - (p_g P_L) \ln (p_g P_L) - (p_e P_L) \ln (p_e P_L) + P_R (p_g - p_e) \ln (p_g / p_e)} \right\} \\ &= 1 - \frac{\Delta}{k_B T \ln (p_g / p_e)} \\ &= 1 - \frac{T_D}{T}, \end{aligned} \quad (23)$$

where the third line follows from the Taylor expansion $(c_1 + c_2 x) \ln (c_1 + c_2 x) = c_1 \ln c_1 + c_2 (\ln c_1 + 1)x + o(x^2)$ with $x \rightarrow 0$ (here c_1 and c_2 are constants), and the last line follows from the definition of $T_D := \Delta / [k_B \ln (p_g / p_e)]$ due to the initial probability distribution $p_g = 1 / (1 + e^{-\beta_D \Delta})$ and $p_e = 1 - p_g$. This result speaks for itself, i.e. one may go beyond the classical Carnot efficiency $\eta_{\text{Carnot}} = 1 - T_D / T$ by consuming a certain amount of quantum coherence, see figure 3. But it is worth stressing that the quantum second law always holds though the classical Carnot bound can be violated, because the bound is defined by the diagonal elements. If we define the Carnot efficiency by considering both the diagonal and off-diagonal elements of QMD, then the total efficiency of the quantum thermodynamic cycle will be limited by this so-called quantum Carnot efficiency.

In particular, there exists a critical probability P_R^{cri} , below which the efficiency goes beyond the classical Carnot efficiency. According to equation (22), P_R^{cri} satisfies $T_D(\Delta S_c + k_B \Delta C_r) = P_R^{\text{cri}}(p_g - p_e)\Delta$, which means QMD's absorption of heat maintains balance with the energy flow of the total composite system. Furthermore, when P_R is larger than a certain value P_R^0 , the efficiency is zero. However, with the increase of coherence, the value of P_R^0 will become higher. This quirk is completely the quantum effect as it depends on how much resource of quantum coherence we expend, in the light of the quantitative resource theory of coherence.

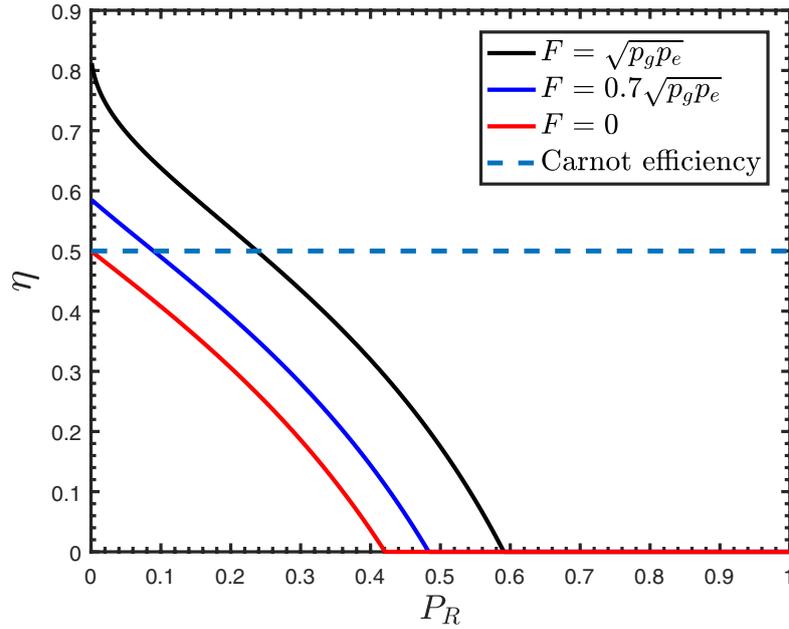


Figure 3. The efficiency η with respect to the quantum probability P_R of finding the system S on the right side for different off-diagonal (coherent) element F . In the classical case, the efficiency must be limited by Carnot efficiency (the red line). However, with the coherence-assisted QMD, this limit may be allowed for a breakthrough (the case of pure state with $F = \sqrt{p_g p_e}$ is depicted by black line and the blue line represents one of the mixed states with $F = 0.7\sqrt{p_g p_e}$). Here we choose $T = 1$, $T_D = 0.5$, $\Delta = 0.5$, and $F = F^*$.

5. Heat engine driven by quantum coherence and general coherence-modified second law

Additionally, we discuss an IHE driven by quantum coherence, which is inspired by [57, 58]. The IHE is constituted by a system S and a reservoir R , which is controlled by a demon consisting of two memories A and B . One can extract work from this IHE by using quantum mutual information, or split into the classical correlation and quantum discord, between these two memories [58]. Then the IHE was generalized to multi-reservoirs case by Ren *et al* who still discussed the work extractable in the same context of quantum discord [57]. Just according to the theme of the present work, a natural question is that whether work can be extracted from the inherent property of one quantum system—coherence, rather than the quantum correlation like discord between two or more systems. We replace the two memories with one memory M in which quantum coherence exists but without any correlations, and investigate the relation between quantum coherence and work extractable from the engine. The schematic diagram of this coherent IHE is briefly shown in figure 4.

Stage (i): Initial state.—Initially, the demon consisting of one memory M is off-line and the system S contacts with the reservoir R at temperature $T = (k_B \beta)^{-1}$ in thermodynamic equilibrium, i.e. the total density matrix of the initial state is expressed as

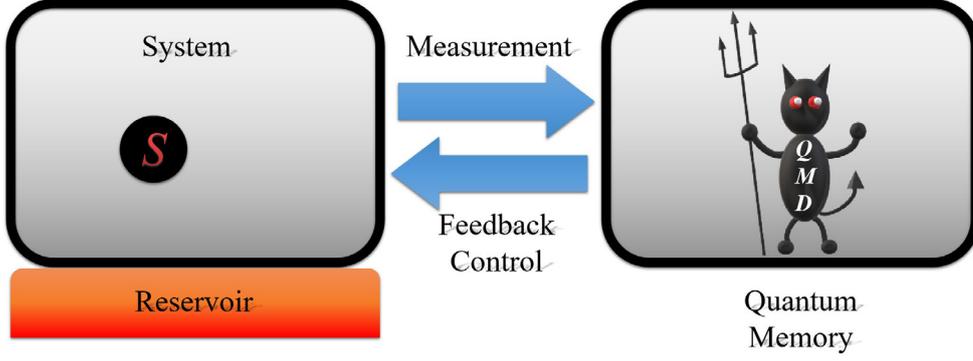


Figure 4. The schematic diagram of the information heat engine driven by quantum coherence.

$$\rho^{(i)} = \rho_M^{(i)} \otimes \rho_{SR}^{(i)} = \rho_M^{(i)} \otimes \frac{e^{-\beta H_S^{(i)}}}{Z_S^{(i)}} \otimes \frac{e^{-\beta H_R}}{Z_R}, \quad (24)$$

where $Z_S^{(i)} = \text{Tr}[e^{-\beta H_S^{(i)}}]$ and $Z_R = \text{Tr}[e^{-\beta H_R}]$ are the initial partition functions of the system S and the reservoir R , respectively. In general, there is no restriction on $\rho_M^{(i)}$.

Stage (ii): Unitary evolution.—The system S begins to interact with R (a unitary evolution), and M is still off-line. Then the density matrix is given by

$$\rho^{(1)} = U^{(1)} \rho^{(i)} U^{(1)\dagger}, \quad (25)$$

with $U^{(1)} = I_M \otimes U_{SR}^{(1)}$. In this stage, the memory still does not participate in the process of IHE.

Stage (iii): POVM.—This stage is where the demon consisting of M started working. The measurement is performed by M with POVMs [1, 25]. Explicitly, the measurement process is implemented by performing a unitary transformation $U^{(2)}$ on the whole system followed by a projection measurement $\{\Pi_M^k : |k\rangle_M \langle k|\}$ (a rank-1 projector) only on M , namely

$$\rho^{(2)} = \sum_k \Pi_M^k U^{(2)} \rho^{(1)} U^{(2)\dagger} \Pi_M^k = \sum_k p_k |k\rangle_M \langle k| \otimes \rho_{SR}^{(2)k}, \quad (26)$$

where $p_k = \text{Tr}[\Pi_M^k U^{(2)} \rho^{(1)} U^{(2)\dagger} \Pi_M^k]$ is the measurement outcome registered by the memory and the postmeasurement state of SR is $\rho_{SR}^{(2)k} = \text{Tr}_A[\Pi_M^k U^{(2)} \rho^{(1)} U^{(2)\dagger} \Pi_M^k / p_k]$.

Stage (iv): Feedback control.—After measurement, the demon will control SR according to the outcome p_k . Mathematically, this feedback control is performed by a unitary operator

$$U^{(3)} = \sum_k |k\rangle_M \langle k| \otimes U_{SR}^k, \quad (27)$$

then the final state becomes

$$\rho^{(f)} = U^{(3)} \rho^{(2)} U^{(3)\dagger}. \quad (28)$$

Note that the final state $\rho^{(f)}$ is not necessarily the canonical distribution, i.e. $\rho_{SR}^{(f)\text{can}} = \exp(-\beta H_S^{(f)}) / Z_S^{(f)} \otimes \exp(-\beta H_R) / Z_R$.

Since the POVMs increases the entropy while the unitary evolution ahead of the measurement keep it invariant, i.e. $S[\rho^{(2)}] \geq S[\rho^{(1)}] = S[U^{(1)}\rho^{(i)}U^{(1)\dagger}] = S[\rho^{(i)}]$, one can obtain

$$S[\rho_{SR}^{(i)}] + S[\rho_M^{(i)}] \leq S[\rho_M^{(2)}] + \sum_k p_k S[\rho_{SR}^{(2)k}] \leq S[\rho_M^{(2)}] + S[\rho_{SR}^{(2)}], \quad (29)$$

where the second inequality follows from the subadditivity of von Neumann entropy [1].

Considering the final state of SR , i.e. $\rho_{SR}^{(f)} = \text{Tr}_M[\rho^{(f)}] = \sum_k U_{SR}^k \rho_{SR}^{(2)k} U_{SR}^{k\dagger}$, we can obtain the following inequality by virtue of the concavity of the von Neumann entropy [1]

$$S[\rho_{SR}^{(f)}] \geq \sum_k p_k S[\rho_{SR}^{(2)k}]. \quad (30)$$

Likewise, we have $\rho_M^{(f)} = \text{Tr}_{SR}[\rho^{(f)}] = \sum_k |k\rangle_M \langle k| = \text{Tr}_{SR}[\rho^{(2)}] = \rho_M^{(2)}$, thus

$$S[\rho_M^{(f)}] = S[\rho_M^{(2)}]. \quad (31)$$

By substituting equations (30) and (31) into equation (29), one obtains

$$S[\rho_{SR}^{(i)}] - S[\rho_{SR}^{(f)}] \leq S[\rho_M^{(f)}] - S[\rho_M^{(i)}], \quad (32)$$

which implies the entropy decrease of the heat engine and the reservoir cannot exceed the entropy increase of the memory, or should say, the whole system satisfies a general principle of entropy increase, i.e. $\Delta S_{SR} + \Delta S \geq 0$, where $\Delta S_{SR} = S[\rho_{SR}^{(f)}] - S[\rho_{SR}^{(i)}]$ and $\Delta S = S[\rho_M^{(f)}] - S[\rho_M^{(i)}]$. According to the quantum version of Klein's inequality, i.e. $\text{Tr}[\rho_{SR}^{(f)} \ln \rho_{SR}^{(f)\text{can}}] \leq \text{Tr}[\rho_{SR}^{(f)} \ln \rho_{SR}^{(i)}]$ [25], equation (32) becomes

$$S[\rho_{SR}^{(i)}] + \text{Tr}[\rho_{SR}^{(f)} \ln \rho_{SR}^{(f)\text{can}}] \leq \Delta S. \quad (33)$$

To investigate the work extractable from the heat engine, we turn the inequality above into the following form by using the canonical distributions $\rho_{SR}^{(i)} = \frac{e^{-\beta H_S^{(i)}}}{Z_S^{(i)}} \otimes \frac{e^{-\beta H_R}}{Z_R}$ and $\rho_{SR}^{(f)\text{can}} = \frac{e^{-\beta H_S^{(f)}}}{Z_S^{(f)}} \otimes \frac{e^{-\beta H_R}}{Z_R}$:

$$\langle E_S^{(i)} \rangle - \langle E_S^{(f)} \rangle + \langle E_R^{(i)} \rangle - \langle E_R^{(f)} \rangle \leq F_S^{(i)} - F_S^{(f)} + k_B T \Delta S \quad (34)$$

with $\langle E_S^{(i)} \rangle = \text{Tr}[\rho_S^{(i)} H_S^{(i)}]$, $\langle E_S^{(f)} \rangle = \text{Tr}[\rho_S^{(f)} H_S^{(f)}]$, $\langle E_R^{(i)} \rangle = \text{Tr}[\rho_R^{(i)} H_R]$, $\langle E_R^{(f)} \rangle = \text{Tr}[\rho_R^{(f)} H_R]$, $F_S^{(i)} = -k_B T \ln Z_S^{(i)}$, and $F_S^{(f)} = -k_B T \ln Z_S^{(f)}$. Here, the definition of the work extractable is $\langle W_{\text{ext}} \rangle := -\langle \Delta E_S \rangle + \langle Q_S \rangle$, where $\langle \Delta E_S \rangle = \langle E_S^{(f)} \rangle - \langle E_S^{(i)} \rangle$ is the change of the internal energy of S and $\langle Q_S \rangle = \langle E_R^{(f)} \rangle - \langle E_R^{(i)} \rangle$ is the heat exchange between S and R , and thus we obtain

$$\langle W_{\text{ext}} \rangle \leq -\Delta F_S + T \Delta S_c + k_B T \Delta C_r, \quad (35)$$

in which $\Delta F_S = F_S^{(f)} - F_S^{(i)}$ is the difference of free energy of the system, $\Delta S_c = k_B \Delta S_{\text{diag}} = k_B S[\rho_{M\text{diag}}^{(f)}] - k_B S[\rho_{M\text{diag}}^{(i)}]$ is the classical entropy change, $\Delta C_r = C_r[\rho_M^{(i)}] - C_r[\rho_M^{(f)}]$ is the coherence consumption of the memory. From equation (35), one can notice that if the contribution of ΔF_S is ignored, the bound of the work extractable is given by the total entropy change of the memory, which is split into the change of incoherent part and coherence consumption. Even if no classical entropy changes, i.e. $\Delta S_c = 0$, we still find the maximum work extractable is given by coherence consumption, namely

$$\langle W_{\text{ext}} \rangle \leq k_B T \Delta C_r, \quad (36)$$

which is also in support of the resource-driven viewpoint, specifically, one can extract work from quantum coherence, a potential quantum physical resource, to drive a heat engine.

6. Extending to more general thermodynamics involving quantum coherence

We consider a general quantum system described as $H|\psi_n\rangle = E_n|\psi_n\rangle$, where H , E_n and $|\psi_n\rangle$ are the Hamiltonian, n th eigenenergy and eigenstate, respectively. Here, the system is not necessarily to be a single system. It might be composed of multiple subsystems. In the energy representation, a general density matrix of this system can be given by

$$\rho = \sum_n P_n |\psi_n\rangle\langle\psi_n| + \sum_{n \neq m} P_{nm} |\psi_n\rangle\langle\psi_m|, \quad (37)$$

then the internal energy of the system can be expressed as

$$\langle E \rangle = \text{Tr}[\rho H] = \sum_n P_n E_n \quad (38)$$

where P_n is the probability distribution of n th energy eigenstate. In equilibrium P_n obeys the canonical distribution. Note that although the density matrix contains off-diagonal part, the internal energy of the system is only connected with the diagonal part due to the energy representation.

From the derivative of $\langle E \rangle$, one obtains $d\langle E \rangle = \sum_n (E_n dP_n + P_n dE_n)$. Here, the previous viewpoint is analogizing it to the classical thermodynamic first law, i.e. $dW_c = -dE_c + dQ_c = -dE_c + TdS_c$, where E_c , W_c , Q_c and S_c are the classical internal energy, work, heat and entropy, respectively. Then, the quantum work can be identified as $d\langle W \rangle = -\sum_n P_n dE_n$ [41–43], and quantum heat is $d\langle Q \rangle = \sum_n E_n dP_n$ associated with TdS_c since the classical entropy S_c is defined as $S_c = -k_B \sum_n P_n \ln P_n$.

Nevertheless, one has already noticed that the classical entropy is actually the von Neumann entropy of diagonal density matrix in energy representation, namely

$$S_c = k_B S(\rho_{\text{diag}}), \quad (39)$$

where k_B is the Boltzmann constant and $\rho_{\text{diag}} = \sum_n \langle\psi_n|\rho|\psi_n\rangle |\psi_n\rangle\langle\psi_n|$ denotes the diagonal part of ρ . Therefore, with the analogy above, this quantum system must have lost part of the information concerning its non-equilibrium (off-diagonal) state. To describe the whole quantum state, the entropy must be the whole $k_B S(\rho)$ instead of $k_B S(\rho_{\text{diag}})$ which contains only the information of equilibrium (diagonal). Hence, combined with equation (1), it is natural to define the quantum heat as

$$\langle Q \rangle = \int_{\rho \rightarrow \sigma} \sum_n E_n dP_n + k_B T \Delta C_r, \quad (40)$$

where $\Delta C_r = C_r(\rho) - C_r(\sigma)$ is the coherence consumption of the system from the initial state ρ to the final state σ . Then the first term of the right-hand side of equation (40) only determined by the diagonal (incoherent) part P_n can be considered as the incoherent heat, i.e. $\langle Q_{\text{incoh}} \rangle = \int_{\rho \rightarrow \sigma} \sum_n E_n dP_n = TS_c = k_B TS(\rho_{\text{diag}})$, and the second term can be understood as the coherent heat, i.e. $\langle Q_{\text{coh}} \rangle = k_B T \Delta C_r$. Thus,

$$\langle Q \rangle = \langle Q_{\text{incoh}} \rangle + \langle Q_{\text{coh}} \rangle, \quad (41)$$

which gives the physical origin of quantum heat: the change of diagonal (incoherent) distribution and the coherence consumption.

By virtue of the definition of quantum heat in equation (40), we can define the quantum work as

$$\langle W \rangle = - \int_{\rho \rightarrow \sigma} \sum_n P_n dE_n + k_B T \Delta C_r, \quad (42)$$

since the first law $\langle \Delta E \rangle = -\langle W \rangle + \langle Q \rangle$. Likewise, the quantum work can be written as

$$\langle W \rangle = \langle W_{\text{incoh}} \rangle + \langle W_{\text{coh}} \rangle, \quad (43)$$

with the incoherent work $\langle W_{\text{incoh}} \rangle = - \int_{\rho \rightarrow \sigma} \sum_n P_n dE_n$ and the coherent work $\langle W_{\text{coh}} \rangle = k_B T \Delta C_r$. So the quantum work can be viewed as the contribution of both the change of energy level under the invariable diagonal (incoherent) distribution and the coherence consumption.

In this way, the total internal energy do not concern the off-diagonal part. However, because the total work can be enhanced due to the coherent superposition, the efficiency of a quantum heat engine thus can be improved in the thermodynamic process involving quantum coherence.

7. Conclusions

In summary, we propose and study quantum thermodynamics by utilizing the resource theory of coherence. Two kinds of quantum heat engines assisted by a coherent QMD are discussed in detail, which are based on QSE and IHE, respectively. The quantum thermodynamic cycle based on QSE is divided into five stages: initial state, insertion, measurement, expansion and removal, which are all described by the evolution of quantum ensembles. We explicitly calculated the total quantum work, heat and the corresponding efficiency of this thermodynamic cycle. From a resource-driven viewpoint, the efficiency can be enhanced due to the coherence consumption of QMD, which is one of our main results.

In addition, we discuss an universal engine driven by quantum coherence based on IHE, which is also to achieve the whole measurement and feedback control through QMD. The maximum work extractable is given by the consumption of quantum coherence, leading to a coherence-modified second law. Consequently, one can extract work from quantum coherence to drive this heat engine even without any classical resources.

Finally, the subtle connection between coherence and fundamental thermodynamic notions is extended to a more general quantum thermodynamics. The quantum work and heat can be naturally redefined as a sum of incoherent and coherent parts by considering the first and second thermodynamic laws. Our results are enlightening for the quantum information processes in thermodynamic systems where the coherent superposition of states cannot be ignored.

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ORCID iDs

Yun-Hao Shi  <https://orcid.org/0000-0003-1130-4280>

Ming-Liang Hu  <https://orcid.org/0000-0002-8750-090X>

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