

Quantum Maxwell's Demon in Thermodynamic Cycles

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We study the physical mechanism of Maxwell's Demon (MD) helping to do extra work in thermodynamic cycles, by describing measurement of position, insertion of wall and information erasing of MD in a quantum mechanical fashion. The heat engine is exemplified with one molecule confined in an infinitely deep square potential inserted with a movable solid wall, while the MD is modeled as a two-level system (TLS) for measuring and controlling the motion of the molecule. It is discovered that the MD with quantum coherence or on a lower temperature than that of the heat bath of the particle would enhance the ability of the whole work substance formed by the system plus the MD to do work outside. This observation reveals that the role of the MD essentially is to drive the whole work substance being off equilibrium, or equivalently working with an effective temperature difference. The elaborate studies with this model explicitly reveal the effect of finite size off the classical limit or thermodynamic limit, which contradicts the common sense on Szilard heat engine (SHE). The quantum SHE's efficiency is evaluated in detail to prove the validity of second law of thermodynamics.

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I. INTRODUCTION

Maxwell's demon (MD) has been a notorious being since its existence could violate the second law of thermodynamics (SLoT) [1, 2]: the MD distinguishes the velocities of the gas molecules, and then controls the motions of molecules to create a difference of temperatures between the two domains. In 1929, Leo Szilard proposed the "one molecular heat engine" (we call Szilard heat engine (SHE)) [3] as an alternative version of heat engine assisted by MD. The MD firstly measures which domain, the single molecule stays in and then gives a command to the system for extracting work according to the measurement results. In a thermodynamic cycle, the molecule seems to extract heat from a single heat bath at temperature T , and thus do work $k_B T \ln 2$ without evoking other changes. This consequence obviously violates the SLoT.

The first revival of the studies of MD is due to the recognition about the trade-off between information and entropy in the MD-controlled thermodynamic cycles. The milestone discovery is the "Landauer principle" [4], which reveals that erasing one bit information from the memory in computing process would inevitably accompany an increasing entropy of the environment. In the SHE, the erasing needs work $k_B T \ln 2$ done by the external agent. It gives a conceptual solution for the MD paradox [5] by considering the MD as a part of the whole work substance, thus the erasing information stored in the demon's memory is necessary to restart a new thermodynamic cycle. This observation about erasing the information of the MD finally saves the SLoT.

The recent revival of the studies of MD is due to the development of quantum information science. The corresponding quantum thermodynamics concerns the quantum heat engines (QHEs) [6, 7] utilizing quantum coherent system serving as the work substance. A quantum work substance is a quantum system off the thermodynamic limit, which perseveres its quantum coherence [8, 9] to some extent, and obviously has

tremendous influence on the properties of QHEs. Especially, when quantum MD is included in the thermodynamical cycle [10–12], the whole work substance formed by the work substance plus MD would be off the thermodynamic limit and possesses some quantum coherence. There are many attempts to generalize the SHE by quantum mechanically approaching the measurement process [11], the motion control [10], the insertion and the expansion process [13]. However, to our best knowledge, a fully quantum approach for all actions in the SHE integrated with a quantum MD intrinsically is still lack. The quantum-classical hybrid description of the SHE may result in some notorious observations about MD assisted thermodynamic process, which seems to challenge the common senses in physics. Therefore, we need a fully quantum theory for the MD-assisted thermodynamics.

In this paper, we propose a quantum SHE assisted by MD with a finite temperature different from that of the system. In this model, we give a consistent quantum approach to the measurement process without using the von Neumann projection [14]. Then we calculate the works done by the insertion of the movable wall in the framework of quantum mechanics. The controlled gas expansion is treated with the quantum conditional dynamics. Furthermore, we also consider the process of removing wall to complete a thermodynamic cycles. With these necessary subtle considerations, the quantum approach for the MD-assisted thermodynamic cycle will go much beyond the conventional theories about the SHE. We show that the system off the thermodynamic limit exhibits uncommon observable quantum effects due to the finite size of system, which results in the discrete energy levels that could be washed out by the heat fluctuation. Quantum coherence can assist the MD to extract more work by reducing effective temperature, while thermal excitation of the MD at a finite temperature would reduce its abilities for quantum measurement and conditional control of the expansion. It means that, only cooled to the absolute zero temperature, could the MD help the molecule to do maximum work outside.

Our paper is organized as follows: In Sec. II we firstly give a brief review of classical version of SHE, and then present our model in quantum version with MD included intrinsically.

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The role of quantum coherence of MD is emphasized with the definition of the effective temperature for arbitrary two level system. In the Sec. III of main part, we consider the quantum SHE with a quantum MD at finite temperature, doing measurement for the position of the particle confined in a one dimensional infinite deep well. The whole cycle consists four steps: insertion, measurement, expansion and removing. Detailed descriptions are performed subsequently in the whole cycle of SHE. We calculate the work done and heat exchange in every sub-step. In Sec. IV, we discuss quantum SHE's operation efficiency in comparison with the Carnot heat engine. We restore the well-known results in the classical case by tuning the parameters in the quantum version, such as the width of the potential well. Conclusions and remarks are given in Sec. VI.

II. QUANTUM MAXWELL'S DEMON IN SZILARD HEAT ENGINE

In this section, we firstly revisit Szilard's single molecular heat engine (SHE) in brief. As illustrated in Fig. 1(a), the whole thermodynamic cycle consists three steps: insertion(i-ii), measurement(ii-iii) and controlled expansion(iii-iv) by the MD. The demon inserts a piston isothermally in the center of the chamber. Then, it finds which domain, the single molecule stays in and changes its own state to register the information of the system. Without losing generality, we assume the demon initially is in the state 0. Finding the molecule is on the right, namely $L/2 < x < L$, the demon changes its own memory to state 1, while it does not change if the molecule is on the left ($0 < x < L/2$). According to the information acquired in the measurement process, the demon controls the expansion of the domain with the single molecule: allowing the isothermal expansion with the piston moving from $L/2$ to L if its memory registers 0, and moving from $L/2$ to 0, if the register is on the state 1. In each thermodynamic cycle, the system does work $W = k_B T \ln 2$ to the outside agent in the isothermal expansion. In an overall looking, the system extracts heat from a single heat bath to do work, thus it would violate the SLot if the MD were not treated as a part of the work substance in the SHE. However, after the cycle, MD stores one bit information as its final state and is in the mixture of 0 and 1 states with equal probability. Thus it does not return to its initial state. Landauer's principle states that to erase such a bit of information at temperature T requires the dissipation of energy at least $k_B T \ln 2$. The work extracted by the system just compensates the energy for erasing the information. Therefore, the SLot is saved. In this sense, the classical version of MD paradox is only a misunderstanding, due to the ignorance of some roles of the MD [5].

In the most of previous investigations about the MD paradox, it is usually assumed the system and the MD possess the same heat bath. Thus the whole work substance formed by the system plus the MD is in equilibrium, and no quantum coherence exists. If the demon is in contact with a lower temperature heat bath while the system's environment possesses higher temperature T , the work needed in the erasing process

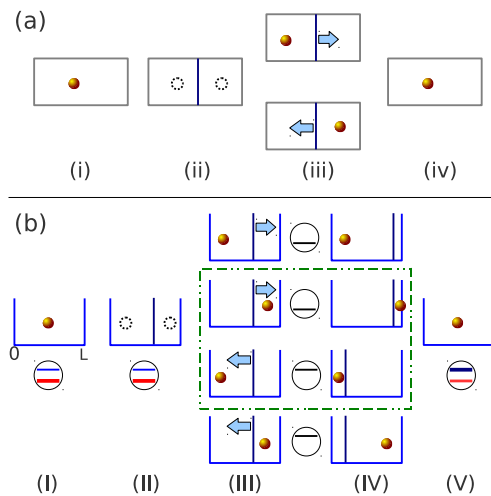


FIG. 1: Classical and quantum Szilard's single molecular heat engine. **(a)** Classical version: (i-ii) A piston is inserted in the center of a chamber. (ii-iii) The demon finds which domain, the single molecule stays in. (iii-iv) The demon controls the system to do work according to its memory; **(b)** Quantum version: The demon is modeled as a two level system with two energy levels $|g\rangle$ and $|e\rangle$ and energy spacing Δ . The chamber is quantum mechanically described as an infinite potential with width L . (I-II) An impenetrable wall is inserted at arbitrary position in the potential. (II-III) The demon measures the state of the system and then record the results in its memory by flipping its own state or no action taken. The measurement may result in the wrong results illustrated in the green dashed rectangle. (III-IV) The demon controls the expansion for the single molecule according to the measurement. (IV-V) The wall is removed from the potential.

is smaller than $k_B T \ln 2$ [10]. Under this circumstance, we actually construct a quantum heat engine with non-equilibrium or an equilibrium working substance work between two different heat baths. Furthermore, when the MD is initially prepared with quantum coherence, the quantum nature of the whole work substance results in many exotic functions for QHE.

To tackle this problem, we study here a quantum version of Szilard's model with an MD accompanying it. In this model, the chamber is modeled as an infinite square potential well with the width L , as illustrated in Fig. 1(b). And the demon is realized by a single two-level atom with energy levels $|g\rangle$, $|e\rangle$ and level spacing Δ . Initially, the system is in thermal state with inverse temperature β . And the demon has been in contact with the low temperature bath at the inverse temperature β_D . Namely, the demon is initial prepared in the equilibrium state

$$\rho_D = p_g |g\rangle\langle g| + p_e |e\rangle\langle e|, \quad (1)$$

with the probability $p_e = 1 - p_g$ in the excited state and one in ground state

$$p_g = 1 / [1 + \exp(-\beta_D \Delta)].$$

Actually, the inverse temperature β_D could represent an effective inverse temperature of the MD with quantum coherence. For an environment being a mesoscopic system, the

number of its degrees of freedom is not so large. Under this circumstance, the strong coupling to the MD leaves finite off-diagonal elements in the reduced density matrix[15]. This remnant of coherence can be utilized to improve the apparent efficiency of the heat engine [8, 9]. For the demon with coherence, the density matrix usually reads as

$$\rho_D = \begin{bmatrix} p_g & F \\ F^* & p_e \end{bmatrix}, \quad (2)$$

where the off-diagonal element F measures the quantum coherence. The eigen-values of the above reduced density matrix represent two effective population probabilities as

$$\begin{aligned} p_+(F) &\approx p_e - \coth\left(\frac{\Delta}{2}\beta_D\right)|F|^2, \\ p_-(F) &\approx p_g + \coth\left(\frac{\Delta}{2}\beta_D\right)|F|^2. \end{aligned} \quad (3)$$

We can define an effective inverse temperature $\beta_{\text{eff}} = \ln p_+(F)/p_-(F)$ for the two-level MD, namely,

$$\beta_{\text{eff}} = \beta_D + \frac{4|F|^2}{\Delta} \cosh^2\left(\frac{\Delta}{2}\beta_D\right) \coth\left(\frac{\Delta}{2}\beta_D\right). \quad (4)$$

The effective temperature $T_{\text{eff}} = 1/\beta_{\text{eff}}$ here is lower than the bath temperature T_D . As shown as follows, it is the lowering of the effective temperature of the MD that results in an increasing of the heat engine efficiency.

As for the modeling of the chamber as an infinite square potential well, the eigenfunctions of the confined single molecule are

$$\langle x | \psi_n(L) \rangle = \sqrt{\frac{2}{L}} \sin[n\pi x/L], \quad (5)$$

with the corresponding eigen-energies $E_n(L) = (\hbar n\pi)^2 / (2mL^2)$, where the quantum number n ranges from 1 to ∞ .

On this bases, the initial state of the total system is expressed as a product state

$$\rho_0 = \frac{1}{Z(L)} \sum_n e^{-\beta E_n(L)} |\psi_n(L)\rangle \langle \psi_n(L)| \otimes \rho_0^D, \quad (6)$$

where

$$Z(L) = \sum_n \exp[-\beta E_n(L)] \quad (7)$$

is the partition function of the system.

Here, we remark that the discrete spectrum of the system results from the finite size of the width L . As $L \rightarrow \infty$, the spectrum becomes continuous as the energy level spacings is proportional to $1/L^2$. Then heat excitation characterized by $k_B T$ can wash out the quantum effect so that the system approaches a classical limit. Some of finite size effect based quantum phenomenon could also disappear as $T \rightarrow \infty$.

With the above modelings, the MD-assisted thermodynamic cycle for the quantum SHE is divided as four steps illustrated in Fig. 1(b): (I-II) the insertion of a mobile solid wall

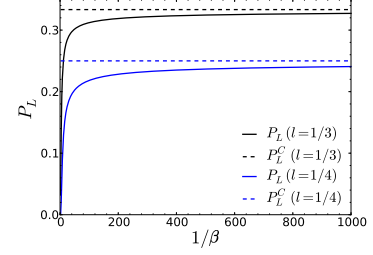


FIG. 2: (Color Online) Probability P_L and the corresponding classical one P_L^C vs temperature $1/\beta$ for different piston position $l = 1/3$ and $l = 1/4$. Without losing generality, we set the parameters as $L = 1$, $m = \pi^2/2$ and $\hbar = 1$.

into the potential well at a position $x = l$ (the origin is $x = 0$); (II-III) the measurement done by the MD to create the quantum entanglement of its two internal states to the spatial wave functions of the confined molecule; (III-IV) quantum control for the mobile wall to move the according to the record in the demon's memory; (IV-V) removing the wall so that the next thermodynamic cycle can be restarted. Their descriptions will be discussed subsequently in the next section and detailed calculations will be found in the Appendix.

III. QUANTUM THERMODYNAMIC CYCLES WITH MEASUREMENT

In this section we analyze in details the thermodynamic cycle of the molecule confined in an infinite square potential well. The molecule's position is monitored and then controlled by the MD. The MD may have quantum coherence as in Eq.2, or equivalently, possesses a lower temperature $T_D = 1/\beta_D$ than $T = 1/\beta$ of the confined molecule's heat bath. In each step, we will evaluate the work done by outside agent and heat exchange in detail. In order to concentrate on the physical properties, we put the calculations in the Appendix.

Step1: Quantum Insertion (I-II)

In the first process, the system is in contact with the heat bath β , then a piston is inserted isothermally into the potential at position l . The potential is then divided into two domains, denoted simply as L and R , with the length l and $L - l$ respectively. The eigenstates change into the following two sets as

$$\langle x | \psi_n^R(L-l) \rangle = \begin{cases} \sqrt{\frac{2}{L-l}} \sin\left[\frac{n\pi(x-l)}{L-l}\right] & l \leq x \leq L \\ 0 & 0 \leq x \leq l \end{cases}, \quad (8)$$

and

$$\langle x | \psi_n^L(l) \rangle = \begin{cases} 0 & l \leq x \leq L \\ \sqrt{\frac{2}{l}} \sin(n\pi x/l) & 0 \leq x \leq l \end{cases},$$

with the corresponding eigen-values $E_n(L-l)$ and $E_n(l)$. In the following discussions we use the free Hamiltonian $H_T = H + H_D$ for

$$H = \sum_n [E_n(l) |\psi_n(l)\rangle \langle \psi_n(l)| + E_n(L-l) |\psi_n(L-l)\rangle \langle \psi_n(L-l)|]$$

for $0 \leq l \leq L$ and $H_D = \Delta |e\rangle \langle e|$. Here, we take its ground state energy as the zero point of energy of atom.

At the end of the insertion process, the system is still in the thermal state with the temperature β and the MD is on its own state without any changes. With respect to the above splitted bases, the state of the whole system is rewritten in terms of the new bases as

$$\rho_{\text{ins}} = [P_L(l) \rho^L(l) + P_R(l) \rho^R(L-l)] \otimes \rho_0^D, \quad (9)$$

where

$$\rho^L(l) = \sum_n \frac{e^{-\beta E_n(l)}}{Z(l)} |\psi_n^L(l)\rangle \langle \psi_n^L(l)|, \quad (10)$$

and

$$\rho^R(L-l) = \sum_n \frac{e^{-\beta E_n(L-l)}}{Z(L-l)} |\psi_n^R(L-l)\rangle \langle \psi_n^R(L-l)|, \quad (11)$$

refer to the system localized in the left and right domain respectively. With respect to their sum $Z(l) = Z(l) + Z(L-l)$, the temperature dependent ratios

$$P_L(l) = Z(l) / Z(l)$$

and

$$P_R(l) = Z(L-l) / Z(l).$$

are the probabilities to find the single molecule on the left and the right side respectively. For simplicity, we denote $P_L(l)$ and $P_R(l)$ by P_L and P_R respectively in the following discussions. We emphasize that the probabilities are different from the classical probabilities, $P_L^c = l/L$ and $P_R^c = (L-l)/L$, finding single molecule on the left and right side that is proportional to the volume. We numerically illustrate this discrepancy between this classical result and ours in Fig. 2 for different insertion position $l = 1/3$ and $l = 1/4$. It is clearly in Fig. 2 that the probabilities P_L approaches to the corresponding classical ones P_L^c , as the temperature increases to the high temperature limit. However, a large discrepancy is observed at low temperature. This deviate from the classical one is due to the discreteness of the energy levels of the potential well with finite width, which disappears as level spacing becomes small with $L \rightarrow \infty$. In this case, the heat excitation will erase

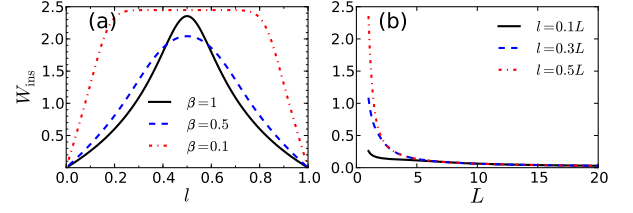


FIG. 3: (Color Online) Work done by the outside agent. (a) W_{ins} vs l for different system inverse temperature $\beta = 1, 0.5$ and 0.1 . Here, we choose the same parameter as that in Fig. 2. (b) W_{ins} vs L for different insertion position $l = 0.1L, 0.3L$ and $0.5L$.

all the quantum feature of the system and the classical limit is approached.

In this step, work should be done to the system. In the isothermal process, the work done by the outside agent can be expressed as $W_{\text{ins}} = \Delta U_{\text{ins}} - T \Delta S_{\text{ins}}$, with the internal energy change

$$\Delta U_{\text{ins}} = \text{Tr}[(\rho_{\text{ins}} - \rho_0) H_T]$$

and the total entropy change

$$\Delta S_{\text{ins}} = \text{Tr}(-\rho_{\text{ins}} \ln \rho_{\text{ins}} + \rho_0 \ln \rho_0).$$

During this isothermal process, the work done by outside just compensates the change of the free energy as

$$W_{\text{ins}} = T [\ln Z(L) - \ln Z(l)]. \quad (12)$$

The same result has been obtained in Ref. [13]. By taken inverse temperature $\beta = 1$ and $L = 1$, we illustrate the work needed for the insertion of the piston into the potential in Fig. 3. It is shown that to insert the piston at the center of the potential needs the maximum work to be done. Another reasonable fact is that no work is needed to insert the piston at position $l = 0$ and $l = L$. Classically, it is well known that no work should be paid for inserting the piston at any position, while for a fixed L , we notice that $W_{\text{ins}} \rightarrow -\infty$ as $T \rightarrow \infty$. The discrete property of the system due to the finite width of the potential well results in the typical quantum effect, even at a high temperature, namely, $\lim_{T \rightarrow \infty} W_{\text{ins}} \neq 0$ and $\lim_{T \rightarrow \infty} Q_{\text{ins}} \neq 0$. This finite size induced quantum effect is typical for mesoscopic system. To restore the classical results, we simply take the limit $L \rightarrow \infty$ to make the spectrum continuous, rather than $T \rightarrow \infty$. Under this limit $L \rightarrow \infty$, we have $Z(l)/Z(L) \rightarrow 1$, which just recovers the classical result that

$$\lim_{L \rightarrow \infty} W_{\text{ins}} = 0, \quad (13)$$

as illustrated in Fig. 3(b) for different insertion positions $l = 0.1L, 0.3L$ and $0.5L$.

After the insertion of piston, the entropy of the system changes. The system exchanges heat with the heat bath during this isothermal reversible process. The heat is obtained by $Q_{\text{ins}} = -T \Delta S_{\text{ins}}$ as

$$Q_{\text{ins}} = \left(T - \frac{\partial}{\partial \beta} \right) [\ln Z(L) - \ln Z(l)]. \quad (14)$$

Similar to the asymptotic properties of the work in Eq. (13), Q_{ins} approaches to zero when $L \rightarrow \infty$.

Step2: Quantum Measurement (II-III)

In the second step, the system is isolated from the heat bath. The MD finds which domain, the single molecule stays in and registers the result into its own memory. In the classical way, the memory can also be imaged as a chamber with single molecule. The classical state of single molecule on the right and left side are denoted as the state 0 and 1. And the memory is architecture always by two bistable states with no energy difference $\Delta = 0$ and no energy is needed in the measurement process. This setup based on ‘‘chamber’’ argument seems to exclude the possibility for quantum coherence in a straightforward way. Therefore, we adopt the TLS as the memory to allow the quantum coherence to take the role, as discussed in Sec. II. In the scheme here, the demon performs the controlled-NOT operation [10]. If the molecule is on the left side, no operation is done. And the demon flips its state, when finding the molecule on the right. This operation is realized by the following unitary operator,

$$U = \sum_n |\psi_n^L(l)\rangle \langle \psi_n^L(l)| \otimes (|g\rangle \langle g| + |e\rangle \langle e|) + |\psi_n^R(L-l)\rangle \langle \psi_n^R(L-l)| \otimes (|e\rangle \langle g| + \text{h.c.}). \quad (15)$$

After the measurement, the MD and the system are correlated. This correlation enables the MD to control the system to perform work to the outside agent. The density matrix of the whole system after measurement is

$$\rho_{\text{mea}} = \left[P_L p_g \rho^L(l) + P_R p_e \rho^R(L-l) \right] \otimes |g\rangle \langle g| + \left[P_L p_e \rho^L(l) + P_R p_g \rho^R(L-l) \right] \otimes |e\rangle \langle e|. \quad (16)$$

If the temperature of the demon is zero, namely $T_D = 0$, the measurement actually results in a perfect correlation between the system and the MD,

$$\rho_{\text{mea}} = P_L \rho^L(l) \otimes |g\rangle \langle g| + P_R \rho^R(L-l) \otimes |e\rangle \langle e|. \quad (17)$$

Then the demon can distinguish exactly the domain where the single molecule stays, e.g. state $|g\rangle$ representing the molecule on left side and vice visa. At a finite temperature, this correlation gets ambiguous. As illustrated in the dashed green box in Fig. 1(b), the demon actually gets the wrong information about the domain, where the single molecule stays. For example, the demon thinks the molecule is on the left with memory registering $|g\rangle$, while the molecule is actually on the right. The MD loses a certain amount of information about the system and lowers its ability to extract work. For case $\Delta \neq 0$ at finite temperature, the above imperfect correlation leads to a condition for the MD’s temperature, under which the total system could extract positive work.

The worst case is that, when we first let the MD to become degenerate, i.e., $\Delta = 0$, then the temperature to approach zero.

In this sense the demon is prepared in a mixing state

$$\rho_0^D(\Delta = 0) = \frac{1}{2} (|g\rangle \langle g| + |e\rangle \langle e|)$$

and the state of the whole system after the measurement reads

$$\rho_{\text{mea}} = \left[\rho^L(l) + \rho^R(L-l) \right] \otimes \rho_0^D(\Delta = 0). \quad (18)$$

Thus, no information is obtained by MD. There exists another limit process that the non-degenerate MD is firstly prepared in the zero-temperature environment, and then let Δ approach zero. Thus, the state of the MD is broken into $|g\rangle \langle g|$ of $\rho_0^D(\Delta = 0)$. In this case, we get a more clever MD as mentioned above. The physical essence of the difference between the two limit processes lies on the symmetry breaking [16] (we will discuss this again later). With such symmetry breaking, the degenerate MD could also make an ideal measurement. A intuitive understanding for the zero-temperature MD helping to do work is that a more calm MD can see the states of the molecule more clear, thus control it more effectively.

Next we calculate the work done in the measurement process by assuming the total system being isolated from the heat bath of the molecule. The heat exchange here is exactly zero, namely $Q_{\text{mea}} = 0$, since the operation is unitary and the total entropy is not changed during this process. However, the total internal energy changes, which merely results from the work done by the outside agent

$$W_{\text{mea}} = P_R (p_g - p_e) \Delta.$$

to register the MD’s memory. The work needed is actually a monotonous function of the demon’s bath temperature T_D . If the temperature of the demon is zero (the MD is prepared in a pure state), namely $T_D = 0$, the work reaches its maximum $W_{\text{mea}}^{\text{max}} = P_R \Delta$. The demon can distinguish exactly the domain, where the single molecule stays, state $|g\rangle$ representing molecule on the left, and vice visa. As discussed as follows, the work done by the outside agent here is the main factor to low down the efficiency of the heat engine. However, the low temperature results in a more perfect quantum correlation between the MD and the system, thus enables the MD to extract more work. Requirement of the work done in the measurement and the ability of controlling free expansion are two competing factors of the QHE. Finally, we prove that a low temperature of the demon results in the high efficiency of quantum heat engine in the following section. It is clear that less work is needed, if the insertion position is closer to the right boundary of the potential. And the work needed in the measurement process approaches to zero, namely $W_{\text{mea}} \rightarrow 0$, when $l \rightarrow L$. Thus, the efficiency is promoted to reach the corresponding Carnot efficiency when $l = L$ for this measurement.

Step3: Controlled Expansion (III-IV)

In the third step, the system is brought into contact with the heat bath with temperature β . Then the expansion is performed slowly enough to enable the process to be reversible

and isothermal. The expansion is controlled by the demon according to its memory. Finding its state on $|g\rangle$, the outside agent allows the piston to move right, thus the single molecule performs work to the outside. However, the agent pays some work to move piston to the right if the MD's memory is inaccurate, e.g. the situation in the green dashed box in Fig. 1(b). If in state $|e\rangle$, the piston is allowed to move to the left side. Under this description, we avoid the conventional heuristic discussion with adding an object in the classical version of SHE. Here, we choose two arbitrary final positions of the controlled expansion as l_g and l_e for the corresponding MD's state $|g\rangle$ and $|e\rangle$. We will prove later that the total work extracted is independent on the expansion position chosen here. After the expansion process, the density matrix of the whole system is expressed as

$$\rho_{\text{exp}} = \left[P_L P_g \rho^L(l_g) + P_R P_e \rho^R(L - l_g) \right] \otimes |g\rangle \langle g| + \left[P_L P_e \rho^L(l_e) + P_R P_g \rho^R(L - l_e) \right] \otimes |e\rangle \langle e|. \quad (19)$$

During the expansion, the system performs work $-W_{\text{exp}} \geq 0$ to the outside agent,

$$W_{\text{exp}} = T \left[\ln Z(l) + P_L \ln P_L + P_R \ln P_R - P_L p_g \ln Z(l_g) - P_R p_e \ln Z(L - l_g) - P_L p_e \ln Z(l_e) - P_R p_g \ln Z(L - l_e) \right]. \quad (20)$$

For a perfect correlation ($p_g = 1$), the piston is moved to the side of the potential, namely $l_g = L$ and $l_e = 0$, and the work is simply

$$W_{\text{exp}} = T (P_L \ln P_L + P_R \ln P_R) - W_{\text{ins}},$$

which is the maximum work one can be extracted in this process. In the classical limit $L \rightarrow \infty$, and the work is

$$W_{\text{exp}} = T (P_L \ln P_L + P_R \ln P_R).$$

We restore the well known result $W_{\text{exp}} = -k_B T \ln 2$, when the piston is inserted in the center of the potential. If the demon is not perfectly correlated to the position of the single molecule ($p_g < 1$), the work extracted $-W_{\text{exp}}$ would be less. Therefore, it is clear that the ability of MD to extract work closely depends on the accuracy of the measurement.

In this step, the heat exchange is related to the change of entropy as

$$Q_{\text{exp}} = P_L \left(T - \frac{\partial}{\partial \beta} \right) \left[\ln Z(l) - p_g \ln Z(l_g) - p_e \ln Z(L - l_e) \right] + P_R \left(T - \frac{\partial}{\partial \beta} \right) \left[\ln Z(L - l) - p_e \ln Z(L - l_g) - p_g \ln Z(l_e) \right]. \quad (21)$$

Step4: Removing(IV-V)

To complete the thermodynamic cycle, the system and the MD should be reset to their own initial states respectively. As

for the system, the piston inserted in the first step should be removed. In the previous studies, this process is neglected, since the measurements are always ideal and the piston is moved to an end boundary of the chamber. Thus no work is required to remove piston. However, in an arbitrary process, we can show the importance of removing piston in the whole cycle. During this process, the system keeps contact with the heat bath with inverse temperature β and the removing is performed isothermally. The density matrix of the total system after removing the piston reads

$$\rho_{\text{rev}} = \sum_n \frac{e^{-\beta E_n(L)}}{Z(L)} |\psi_n(L)\rangle \langle \psi_n(L)| \otimes \left[(P_L P_g + P_R P_e) |g\rangle \langle g| + (P_L P_e + P_R P_g) |e\rangle \langle e| \right]. \quad (22)$$

In this process, the work done and the heat absorbed by the outside are

$$W_{\text{rev}} = \text{Tr} \left[(\rho_{\text{rev}} - \rho_{\text{exp}}) (H + H_D) \right] - T \text{Tr} \left[-\rho_{\text{rev}} \ln \rho_{\text{rev}} \right] + T \text{Tr} \left[-\rho_{\text{exp}} \ln \rho_{\text{exp}} \right], \quad (23)$$

and

$$Q_{\text{rev}} = -T \text{Tr} \left[-\rho_{\text{rev}} \ln \rho_{\text{rev}} \right] + T \text{Tr} \left[-\rho_{\text{exp}} \ln \rho_{\text{exp}} \right], \quad (24)$$

respectively. We refer the Appendix for the exact expression of those two formula. The MD now is no longer entangled with the system. And the density matrix of the demon is factorized out as

$$\rho_{\text{rev}}^D = (P_L P_g + P_R P_e) |g\rangle \langle g| + (P_L P_e + P_R P_g) |e\rangle \langle e|. \quad (25)$$

In the ideal case $T_D = 0$, the demon is on the state

$$\rho_{\text{rev}}^D = P_L |g\rangle \langle g| + P_e |e\rangle \langle e|$$

with entropy

$$S_{\text{rev}}^D = -P_L \ln P_L - P_e \ln P_e.$$

According to Landauer's Principal, erasing the memory of the MD dissipates at least $T_D S_{\text{rev}}^D = 0$ work into the environment. In this sense, we can extract $k_B T \ln 2$ work with MD's help. However, we does not violate the SLoT, since the whole system functionalizes as a heat engine working between high temperature bath and zero temperature bath. Actually, the increase of entropy in the zero temperature bath is exactly S_{rev}^D . Therefore, the energy dissipated actually depends on the temperature of environment, where the information is erased. In the previous studies, people always set the same temperature for the system and MD. Thus the exactly mechanism of MD was not clear to certain extent, especially for SHE. Let's consider another special case $\Delta = 0$, which directly results in $p_e = p_g = 1/2$. MD is prepared on its maximum entropy state ρ_0^D ($\Delta = 0$). At the end of the cycle, MD actually is on the same state, namely $\rho_{\text{rev}}^D = \rho_0^D$ ($\Delta = 0$). Thus, no work is paid to erase the memory.

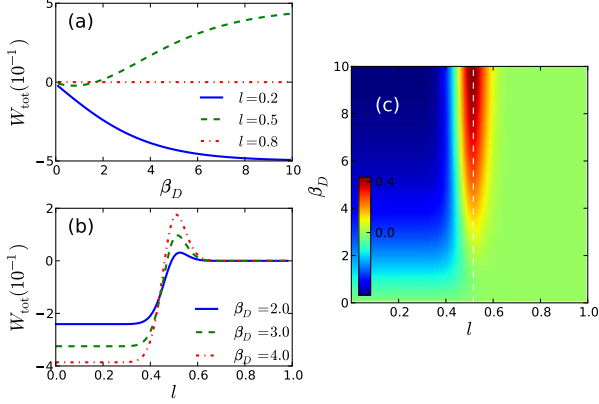


FIG. 4: (Color Online) Work vs insertion position l and MD's inverse temperature β_D . (a) Total work as a function of β_D for different $l = 0.2, 0.5$ and 0.8 . (b) Total work as a function of insertion position l for different $\beta_D = 2.0, 3.0$ and 4.0 . (c) Contour plot for total work as function of l and β_D . The position for maximum work extracted is denoted as white dashed line.

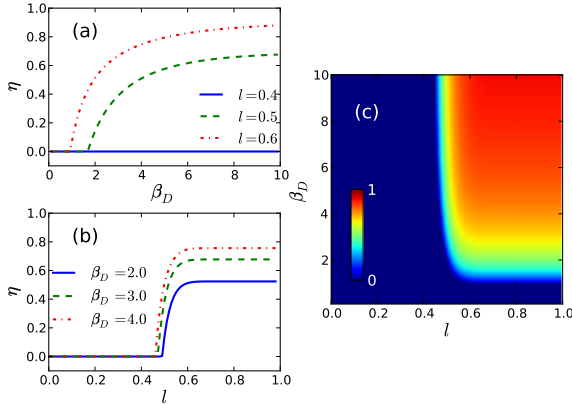


FIG. 5: (Color Online) Efficiency vs insertion position l and O inverse temperature β_D . (a) Efficiency as a function of β_D for different $l = 0.4, 0.5$ and 0.6 . (b) Efficiency as a function l for different $\beta_D = 2, 3$ and 4 . (c) Contour plot of efficiency vs l and β_D .

After this procedure, the MD is decoupled from the system and brought into contact with its own thermal bath with inverse temperature β_D . Since

$$P_L p_e + P_R p_g \geq p_e, \quad (26)$$

the MD releases energy into its heat bath. We will not discuss this thermalization process here in details. The MD and the system are reset to their own initial states ρ_0 , which allows a new cycle to start.

IV. EFFICIENCY OF SZILARD HEAT ENGINE

For quantum version of the SHE, the quantum coherent based on the finite size of the chamber results in various different properties from the classical one. Work is required during the insertion and removing processes, while the same process can be done freely in the classical version. The microscopic model here relates the efficiency of the measurement by MD to the temperature of the heat bath. In the whole thermodynamic cycle, the work done by the system to outside is the sum of all the work done in each process,

$$\begin{aligned} W_{\text{tot}} &= -(W_{\text{ins}} + W_{\text{mea}} + W_{\text{exp}} + W_{\text{rev}}) \\ &= T \left[(p_e \ln p_e + p_g \ln p_g) \right. \\ &\quad - (P_L p_g + P_R p_e) \ln (P_L p_g + P_R p_e) \\ &\quad - (P_L p_e + P_R p_g) \ln (P_L p_e + P_R p_g) \left. \right] \\ &\quad - P_R (p_g - p_e) \Delta. \end{aligned} \quad (27)$$

To enable the system to do work outside, the temperature of the MD should be low enough to make sure $W_{\text{tot}} \geq 0$, which is known as the positive-work condition (PWC) [7]. To evaluate the efficiency of QHE, we need to obtain the heat absorbed from the high temperature heat bath. Different from the classical one, the exchange of heat with high temperature source persists in each step. The total heat absorbed from the high temperature source is the sum over that of all the four steps,

$$\begin{aligned} Q_{\text{tot}} &= -(Q_{\text{ins}} + Q_{\text{mea}} + Q_{\text{exp}} + Q_{\text{rev}}) \\ &= T \left[(p_e \ln p_e + p_g \ln p_g) \right. \\ &\quad - (P_L p_g + P_R p_e) \ln (P_L p_g + P_R p_e) \\ &\quad - (P_L p_e + P_R p_g) \ln (P_L p_e + P_R p_g) \left. \right]. \end{aligned} \quad (28)$$

Here, the absorbed energy is used to perform work to the outside, while only the measurement process wastes W_{mea} , which is released to the low temperature heat bath. It is very interesting to notice that $W_{\text{mea}} \rightarrow 0$ as $\Delta \rightarrow 0$, while the total heat $Q_{\text{tot}} \rightarrow 0$ and $W_{\text{tot}} \rightarrow 0$. To check the validity of SLot, one should concern the the efficiency of this heat engine in a cycle,

$$\eta = 1 - \frac{P_R (p_g - p_e) \Delta}{Q_{\text{tot}}}. \quad (29)$$

As an example, we consider the special case $l = L/2$, which is similar to the case of the ordinary SHE with the piston inserted in the center of the chamber. In this special case, the probabilities for the single molecule staying at the two sides are the same as that of the classical one, namely $P_L = P_R = 1/2$. The total work extracted here can be written in a simple form

$$W_{\text{tot}} = T (\ln 2 + p_e \ln p_e + p_g \ln p_g) - (p_g - p_e) \Delta / 2. \quad (30)$$

In this special case, to make the system capable to do work on the outside, there is a requirement to the temperature of the

demon (low temperature bath). For example, when we choose $\beta = 1$ and $\Delta = 0.5$, the PWC is $\beta_D \geq 2.09$. This requirement is more strict than that of Carnot heat engine, $\beta_D > 1$. And the efficiency of this heat engine reads

$$\eta = 1 - \frac{(p_g - p_e)\Delta}{2T(\ln 2 + p_e \ln p_e + p_g \ln p_g)}, \quad (31)$$

which is lower than the corresponding Carnot efficiency

$$\eta_{\text{Carnot}} = 1 - \frac{T_D}{T}.$$

Here, the efficiency is a monotonic function of the energy spacing Δ and reaches its maximum

$$\eta_{\text{max}} = 1 - \frac{2T_D}{T} \leq \eta_{\text{Carnot}}$$

with $\Delta = 0$.

In the general case, we show the work done by the system and efficiency of the heat engine vs the position of the wall l and the temperature of demon β_D in Fig. 4 and Fig. 5. As illustrated in Fig. 4(a), for small insertion position, e.g. $l = 0.16$ and 0.36 , the system can not extract positive work. There exists a critical insertion position l_{cri} to extract positive work, namely

$$T(P_L^{\text{cri}} \ln P_L^{\text{cri}} + P_R^{\text{cri}} \ln P_R^{\text{cri}}) + P_R^{\text{cri}} \Delta = 0, \quad (32)$$

where $P_R^{\text{cri}} = P_R(l_{\text{cri}})$ and $P_L^{\text{cri}} = P_L(l_{\text{cri}})$. This critical value of insertion position here is $l_{\text{cri}} = 0.447$ for the typical parameter chosen here. Due to the requirement of work in the measurement process, the work extracted is not a symmetric function of the insertion piston l , namely $W_{\text{tot}}(0.5 - l) \neq W_{\text{tot}}(0.5 + l)$, as illustrated in Fig. 4(b,c). Since the high energy state $|e\rangle$ of the demon is utilized to register the right side for single molecule, more work is need when $l < L/2$. Due to the requirement of work done by outside agent in the measurement process, the optimal position to extract maximum work is not at the center of the potential. The maximum work can be extracted for a given MD's inverse temperature is reached, when

$$\frac{P_L^{\text{wmax}} p_e + P_R^{\text{wmax}} p_g}{P_L^{\text{wmax}} p_g + P_R^{\text{wmax}} p_e} = e^{-\beta \Delta}, \quad (33)$$

where $P_L^{\text{wmax}} = P_L(l_{\text{wmax}})$ and $P_R^{\text{wmax}} = P_R(l_{\text{wmax}})$. It is clear that the position for the maximum work depends on the temperature of the demon β_D .

In Fig. 5, we show the efficiency of this single molecular heat engine. We consider only the positive work situation, and set efficiency as 0 for all the negative work area. Fig. 5(a) shows the monotonous behavior of efficiency as the MD's inverse temperature. Efficiency is also a monotonous function of the insertion position l , illustrated in Fig. 5(b,c), which is not similar to the total work extracted. It worth noticing that the efficiency reaches its maximum at $l = 1$, while no work can be extracted. Since the measurement is the only way of wasting energy, it is the only way to improve

the efficiency by reducing W_{mea} with decreasing P_R . The efficiency of QHE reaches the well-known Carnot efficiency η_{Carnot} , when $P_R = 0$. At the same time, the total work extracted approaches to zero, namely $W_{\text{tot}} = 0$. We meet this dilemma, since the measurement results in an imperfect correlation between MD and the system.

Before concluding this paper, we draw our attention to two limit processes[16] again

$$\lim_{\beta_D \rightarrow +\infty} \lim_{\Delta \rightarrow 0} \rho_D = (|g\rangle\langle g| + |e\rangle\langle e|)/2, \quad (34)$$

$$\lim_{\Delta \rightarrow 0} \lim_{\beta_D \rightarrow +\infty} \rho_D = |g\rangle\langle g|. \quad (35)$$

Note that taking the two limits in different orders leads to completely different results, the latter being a reflection of the spontaneous symmetry breaking phenomenon. This difference for the MD's initial state results in the different work extracted, namely,

$$\lim_{\beta_D \rightarrow +\infty} \lim_{\Delta \rightarrow 0} W_{\text{tot}} = 0, \quad (36)$$

$$\lim_{\Delta \rightarrow 0} \lim_{\beta_D \rightarrow +\infty} W_{\text{tot}} = k_B T \ln 2. \quad (37)$$

The former one means that MD actually gets no information about the position of molecule and extracts no work, while the latter one show that MD obtains the exact information on the position of the molecule and enables the system to perform maximum work to the outside agent. The same phenomenon has also been revealed in the process of dynamic thermalization[16].

V. CONCLUSIONS

In summary, we have studied a quantum version of SHE with a quantum MD with lower finite temperature than that of the system. We overall simplified the MD as a two-level system, which carries out measurement in quantum fashion and controlling the system to do work to the out-side agent. In this sense, the MD assisted thermodynamic cycle are clarified as the four steps, insertion, measurement, expansion and removing, which are all described in the framework of quantum mechanics. In each step, we also consider the special case to restore the well-known results in classical version of SHE. We explicitly analyzed the total work extracted and the corresponding efficiency. To resolve the MD paradox, we compared the obtained efficiency of the heat engine with that of Carnot heat engine. It is found the efficiency is always below that of Carnot since the quantum MD is included as the a part of the the whole work substance and its functions are also correctly "quantized". Thus nothing violates the SLoT.

In comparison with the classical version of SHE, the following quantum natures were discovered in the quantum thermodynamic cycles: (1) The finite size effect of the potential well was found as reason for the non-vanishing work required in the insertion and removing of the middle walls, while the corresponding manipulations could be achieved freely in the classical case; (2) The quantum coherence is allowed to exist

in the MD's density matrix. It is the decrease of effective temperature caused by this coherence that actually improves the efficiency of SHE; (3) In the measurement process, the finite temperature of MD actually results in the incorrect decision to control the single molecule's motion. This incorrectness decreased the MD's ability to extract work. To our best knowledge, even for in the classical case, the similar investigation has never been carried out; (4) In the whole thermodynamic cycle, the removing process is necessary in returning to the initial state for the whole work substance. This fact is neglected in the previous studies even for the classical SHE.

Finally, we should stress that the model studied here could help to resolve many paradoxical observations due to heuristic arguments with hybridization of classical-quantum points of views about thermodynamics. For instance, it could be recognized that the conventional argument about the MD paradox only concerns a classical version of MD at the same temperature as that of the system. Our results can enlighten the comprehensive understandings about some fundamental problems in thermodynamics, such as the relationship between quantum unitarity and SLoT[17].

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Appendix

In this appendix, we present a detailed calculation for the work done and efficiency of SHE. Following the calculations for the four steps listed in the context step by step, the reader can deeply understand the physical essences of the MD in some subtle fashion.

Step 1: Insertion. In this process, the changes of internal energy $\Delta U_{\text{int}} = \text{Tr}[(H + H_D)(\rho_{\text{ins}} - \rho_0)]$ and total entropy $\Delta S_{\text{ins}} = \text{Tr}[-\rho_{\text{ins}} \ln \rho_{\text{ins}}] - \text{Tr}[-\rho_0 \ln(\rho_0)]$ is explicitly given by

$$\begin{aligned} \Delta U_{\text{int}} &= \sum_n p_n(l) E_n(l) + \\ &\sum_n p_n(l') E_n(l') - \sum_n p_n(L) E_n(L) \quad (38) \\ &= \frac{\partial}{\partial \beta} [\ln Z(L) - \ln Z(l)], \end{aligned}$$

where $L' = L - l$ and

$$\begin{aligned} \Delta S_{\text{ins}} &= (\ln Z(l) - \ln Z(L)) + \\ &\beta \sum_n \left[\begin{array}{c} p_n(l) E_n(l) \\ + p_n(l') E_n(l') - p_n(L) E_n(L) \end{array} \right] \\ &= \left(1 - \beta \frac{\partial}{\partial \beta} \right) (\ln Z(l) - \ln Z(L)), \quad (39) \end{aligned}$$

where

$$p_n(y) = \frac{\exp(-\beta E_n(y))}{Z(y)}.$$

For the isothermal process, the work done by outside agent and the heat exchange are simply $W_{\text{ins}} = \Delta U_{\text{int}} - T \Delta S_{\text{ins}}$ and $Q_{\text{ins}} = -T \Delta S_{\text{ins}}$, namely,

$$W_{\text{ins}} = T [\ln Z(L) - \ln Z(l)], \quad (40)$$

$$Q_{\text{ins}} = \left(T - \frac{\partial}{\partial \beta} \right) [\ln Z(L) - \ln Z(l)]. \quad (41)$$

Step2: Measurement. The measurement is realized by a controlled-NOT unitary operation, which has been illustrated clearly in the Sec. II. After the measurement process, the density matrix for the total system is

$$\begin{aligned} \rho_{\text{mea}} &= \left[P_L p_g \rho^L(l) + P_R p_e \rho^R(l') \right] \otimes |g\rangle \langle g| \\ &+ \left[P_L p_e \rho^L(l) + P_R p_g \rho^R(l') \right] \otimes |e\rangle \langle e|. \end{aligned}$$

The entropy is not changed in this step. And the work done by outside is

$$W_{\text{mea}} = \Delta U_{\text{mea}} = P_R (p_g - p_e) \Delta. \quad (42)$$

Step3: Controlled expansion. At the ending of expansion, the state for the total system reads

$$\begin{aligned} \rho_{\text{exp}} &= \left[P_L p_g \rho^L(l_g) + P_R p_e \rho^R(l_e) \right] \otimes |g\rangle \langle g| \\ &+ \left[P_L p_e \rho^L(l_e) + P_R p_g \rho^R(l_g) \right] \otimes |e\rangle \langle e|. \end{aligned}$$

where $L_g = L - l_g$ and $L_e = L - l_e$

We move the wall isothermally. And the work done by outside agent can be obtain by the same methods used in insertion process as

$$\begin{aligned}
W_{\text{exp}} &= \text{Tr}[\rho_{\text{exp}}(H + H_D)] - \text{Tr}[\rho_{\text{mea}}(H + H_D)] \\
&\quad - T \text{Tr}[-\rho_{\text{exp}} \ln \rho_{\text{exp}}] + T \text{Tr}[-\rho_{\text{mea}} \ln \rho_{\text{mea}}] \\
&= \sum_n [P_L p_g p_n(l_g) E_n(l_g) + P_R p_e p_n(L_g) E_n(L_g) + P_L p_e p_n(L_e) E_n(L_e) \\
&\quad + P_R p_g p_n(l_e) E_n(l_e)] + (P_L p_e + P_R p_g) \Delta \\
&\quad - \sum_n (P_L p_n(l) E_n(l) + P_R p_n(L') E_n(L')) + (P_L p_e + P_R p_g) \Delta \\
&\quad - T \sum_n [P_L p_g p_n(l_g) \ln P_L p_g p_n(l_g) + P_R p_e p_n(L') \ln P_R p_e p_n(L') \\
&\quad \quad + P_L p_e p_n(L_e) \ln P_L p_e p_n(L_e) + P_R p_g p_n(l_e) \ln P_R p_g p_n(l_e)] \\
&\quad - T \sum_n [p_g p_n(l) \ln p_g p_n(l) + p_e p_n(L') \ln p_e p_n(L') \\
&\quad \quad + p_e p_n(l) \ln p_e p_n(l) + p_g p_n(L') \ln p_g p_n(L')] \\
&= P_L T [\ln Z(l) - p_g \ln Z(l_g) - p_e \ln Z(L_e)] + P_R T [\ln Z(L') - p_e \ln Z(L_g) - p_g \ln Z(l_e)]. \tag{43}
\end{aligned}$$

The internal energy changes can be also evaluated as

$$\begin{aligned}
\Delta U_{\text{exp}} &= \sum_n [P_L p_g p_n(l_g) E_n(l_g) + P_R p_e p_n(L_g) E_n(L_g) + P_L p_e p_n(L_e) E_n(L_e) + P_R p_g p_n(l_e) E_n(l_e)] \\
&\quad + (P_L p_e + P_R p_g) \Delta \\
&\quad - \sum_n (P_L p_n(l) E_n(l) + P_R p_n(L') E_n(L')) + (P_L p_e + P_R p_g) \Delta \\
&= \sum_n [P_L p_g p_n(l_g) E_n(l_g) + P_R p_e p_n(L_g) E_n(L_g) + P_L p_e p_n(L_e) E_n(L_e) + P_R p_g p_n(l_e) E_n(l_e)] \\
&\quad - \sum_n [P_L p_n(l) E_n(l) + P_R p_n(L') E_n(L')] \\
&= P_L \frac{\partial}{\partial \beta} [\ln Z(l) - p_g \ln Z(l_g) - p_e \ln Z(L_e)] + P_R \frac{\partial}{\partial \beta} [\ln Z(L') - p_e \ln Z(L_g) - p_g \ln Z(l_e)]. \tag{45}
\end{aligned}$$

Then, we obtain the heat exchanges in this process as $Q_{\text{exp}} = -T \Delta S_{\text{exp}} = W_{\text{exp}} - \Delta U_{\text{exp}}$ or

$$\begin{aligned}
Q_{\text{exp}} &= P_L \left(T - \frac{\partial}{\partial \beta} \right) [\ln Z(l) - p_g \ln Z(l_g) - p_e \ln Z(L_e)] \\
&\quad + P_R \left(T - \frac{\partial}{\partial \beta} \right) [\ln Z(L') - p_e \ln Z(L_g) - p_g \ln Z(l_e)].
\end{aligned}$$

Step4: Removing. The piston is removed in this process. After that, the system returns to its initial state and is not entangled with MD as The last step would be remove the wall in

the trap. The system is on the state as

$$\rho_{\text{rev}} = \sum_n \frac{\exp[-\beta E_n(L)]}{Z(L)} |\psi_n(L)\rangle \langle \psi_n(L)| \otimes \left[(P_L p_g + P_R p_e) |g\rangle \langle g| + (P_L p_e + P_R p_g) |e\rangle \langle e| \right]. \tag{46}$$

Then, the work done and the heat absorbed is respectively

$$\begin{aligned}
W_{\text{rev}} &= \text{Tr}[\rho_{\text{rev}}(H + H_D)] - \text{Tr}[\rho_{\text{exp}}(H + H_D)] \\
&\quad - T \text{Tr}[-\rho_{\text{rev}} \ln \rho_{\text{rev}}] + T \text{Tr}[-\rho_{\text{exp}} \ln \rho_{\text{exp}}]
\end{aligned} \tag{47}$$

or

$$\begin{aligned}
W_{\text{rev}} &= \sum_n p_n(L) E_n(L) + (P_L p_e + P_R p_g) \Delta \\
&\quad - \sum_n [P_L p_g p_n(l_g) E_n(l_g) + P_R p_e p_n(L_g) E_n(L_g) + P_L p_e p_n(L_e) E_n(L_e) + P_R p_g p_n(l_e) E_n(l_e)] \\
&\quad - (P_L p_e + P_R p_g) \Delta \\
&\quad + T \left[\sum_n p_n(L) \ln p_n(L) + (P_L p_g + P_R p_e) \ln (P_L p_g + P_R p_e) + (P_L p_e + P_R p_g) \ln (P_L p_e + P_R p_g) \right] \\
&\quad - T \sum_n \{ P_L p_g p_n(l_g) \ln [P_L p_g p_n(l_g)] + P_R p_e p_n(L_g) \ln [P_R p_e p_n(L_g)] \\
&\quad \quad + P_L p_e p_n(L_e) \ln [P_L p_e p_n(L_e)] + P_R p_g p_n(l_e) \ln [P_R p_g p_n(l_e)] \} \\
&= T \left[-\ln Z(L) + (P_L p_g + P_R p_e) \ln (P_L p_g + P_R p_e) + (P_L p_e + P_R p_g) \ln (P_L p_e + P_R p_g) \right. \\
&\quad \quad - P_L \ln P_L - P_R \ln P_R - p_e \ln p_e - p_g \ln p_g \\
&\quad \quad \left. + P_L p_g \ln Z(l_g) + P_R p_e \ln Z(L_g) + P_L p_e \ln Z(L_e) + P_R p_g \ln Z(l_e) \right]. \tag{48}
\end{aligned}$$

and

$$\begin{aligned}
Q_{\text{rev}} &= -T \text{Tr} [-\rho_{\text{rev}} \ln \rho_{\text{rev}}] + T \text{Tr} [-\rho_{\text{exp}} \ln \rho_{\text{exp}}] \\
&= T \left[\sum_n p_n(L) \ln p_n(L) + (P_L p_g + P_R p_e) \ln (P_L p_g + P_R p_e) + (P_L p_e + P_R p_g) \ln (P_L p_e + P_R p_g) \right] \\
&\quad - T \sum_n \{ P_L p_g p_n(l_g) \ln [P_L p_g p_n(l_g)] + P_R p_e p_n(L_g) \ln [P_R p_e p_n(L_g)] \\
&\quad \quad + P_L p_e p_n(L_e) \ln [P_L p_e p_n(L_e)] + P_R p_g p_n(l_e) \ln [P_R p_g p_n(l_e)] \} \\
&= T \left\{ -\ln Z(L) + (P_L p_g + P_R p_e) \ln (P_L p_g + P_R p_e) + (P_L p_e + P_R p_g) \ln (P_L p_e + P_R p_g) \right. \\
&\quad \quad \left. - P_L \ln P_L - P_R \ln P_R - p_e \ln p_e - p_g \ln p_g + P_L p_g \ln Z(l_g) + P_R p_e \ln Z(L_g) + P_L p_e \ln Z(L_e) + P_R p_g \ln Z(l_e) \right\} \\
&\quad - \sum_n [p_n(L) E_n(L) - P_L p_g p_n(l_g) E_n(l_g) - P_R p_e p_n(L_g) E_n(L_g) \\
&\quad \quad - P_L p_e p_n(L_e) E_n(L_e) - P_R p_g p_n(l_e) E_n(l_e)] \\
&= T \left[(P_L p_g + P_R p_e) \ln (P_L p_g + P_R p_e) + (P_L p_e + P_R p_g) \ln (P_L p_e + P_R p_g) - P_L \ln P_L - P_R \ln P_R - p_e \ln p_e - p_g \ln p_g \right] \\
&\quad - \left(T - \frac{\partial}{\partial \beta} \right) \ln Z(L) + P_L p_g \left(T - \frac{\partial}{\partial \beta} \right) \ln Z(l_g) + P_R p_e \left(T - \frac{\partial}{\partial \beta} \right) \ln Z(L_g) \\
&\quad + P_L p_e \left(T - \frac{\partial}{\partial \beta} \right) \ln Z(L_e) + P_R p_g \left(T - \frac{\partial}{\partial \beta} \right) \ln Z(l_e). \tag{49}
\end{aligned}$$

The total work extracted by outside agent is the sum of work extracted in each step as

$$\begin{aligned}
W_{\text{tot}} &= -(W_{\text{ins}} + W_{\text{mea}} + W_{\text{exp}} + W_{\text{rev}}) \\
&= T [(p_e \ln p_e + p_g \ln p_g) - (P_L p_g + P_R p_e) \ln (P_L p_g + P_R p_e) \\
&\quad - (P_L p_e + P_R p_g) \ln (P_L p_e + P_R p_g)] - P_R (p_g - p_e) \Delta. \tag{50}
\end{aligned}$$

The total heat absorbed can also be obtained as

$$\begin{aligned}
Q_{\text{tot}} &= -(Q_{\text{ins}} + Q_{\text{exp}} + Q_{\text{rev}}) \\
&= T \left[\begin{aligned} &(p_e \ln p_e + p_g \ln p_g) \\ &- (P_L p_g + P_R p_e) \ln (P_L p_g + P_R p_e) \\ &- (P_L p_e + P_R p_g) \ln (P_L p_e + P_R p_g) \end{aligned} \right]. \tag{51}
\end{aligned}$$

[1] *Maxwell's Demon 2: Entropy, Classical and Quantum Information, Computing*, edited by H. S. Leff and A. F. Rex (Institute

of Physics, Bristol, 2003).

- [2] K. Maruyama, F. Nori, and V. Vedral, *Rev. Mod. Phys.* **81**, 1 (2009).
- [3] L. Szilard, *Z. Phys.* **53**, 840 (1929).
- [4] R. Landauer, *IBM J. Res. Dev.* **5**, 183 (1961).
- [5] C. H. Bennett, *Int. J. Theor. Phys.* **21**, 905 (1982); *Sci. Am.* **257**, 108 (1987).
- [6] T. D. Kieu, *Phys. Rev. Lett.* **93**, 140403 (2004); *Eur. Phys. J. D* **39**, 115 (2006);
- [7] H. T. Quan, Yu-xi Liu, C. P. Sun, and F. Nori, *Phys. Rev. E* **76**, 031105 (2007); H. T. Quan, *Phys. Rev. E* **79**, 041129 (2009).
- [8] M. O. Scully, M. S. Zubairy, G. S. Agarwal, and H. Walther, *Science* **299**, 862 (2003).
- [9] H. T. Quan, P. Zhang, and C. P. Sun, *Phys. Rev. E* **73**, 036122 (2006).
- [10] H. T. Quan, Y. D. Wang, Yu-xi Liu, C. P. Sun, and F. Nori, *Phys. Rev. Lett.* **97**, 180402 (2006).
- [11] W. H. Zurek, Szilard's engine, Maxwell's demon and quantum measurements, lecture notes from NATO ASI in Santa Fe, New Mexico, June 3-17, 1984, pp. 145-150 in the Proceedings *Frontiers of Nonequilibrium Quantum Statistical Mechanics*, edited by G. T. Moore and M. O. Scully (Plenum, 1986).
- [12] S. Lloyd, *Phys. Rev. A* **56**, 3374 (1997).
- [13] S. W. Kim, T. Sagawa, S. D. Liberato, M. Ueda, arXiv:1006.1471 (2010).
- [14] P. Zhang, X. F. Liu, and C. P. Sun, *Phys. Rev. A* **66**, 042104 (2002).
- [15] H. Dong, S. Yang, X.F. Liu and C.P. Sun, *Phys. Rev. A* **76**, 044104 (2007).
- [16] Jie-Qiao Liao, H. Dong, X. G. Wang, X. F. Liu, C. P. Sun, arXiv:0909.1230.
- [17] H. Dong, D.Z. Xu and C. P. Sun, in preparation.