

Quantum Maxwell's demon in thermodynamic cycles

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We study the physical mechanism of Maxwell's demon (MD), which helps do extra work in thermodynamic cycles with the heat engine. This is exemplified with one molecule confined in an infinitely deep square potential with a movable solid wall. The MD is modeled as a two-level system (TLS) for measuring and controlling the motion of the molecule. The processes in the cycle are described in a quantum fashion. It is discovered that a MD with quantum coherence or one at a temperature lower than the molecule's heat bath can enhance the ability of the whole working substance, formed by the heat engine plus the MD, to do work outside. This observation reveals that the essential role of the MD is to drive the whole working substance off equilibrium, or equivalently, to work between two heat baths with different effective temperatures. The elaborate studies with this model explicitly reveal the effect of finite size off the classical limit or thermodynamic limit, which contradicts common sense on a Szilard heat engine (SHE). The quantum SHE's efficiency is evaluated in detail to prove the validity of the second law of thermodynamics.

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I. INTRODUCTION

Maxwell's demon (MD) is notorious 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" (which we call the Szilard heat engine, SHE) [3] as an alternative version of a heat engine assisted by the MD. The MD first measures which domain the single molecule stays in and then manipulates the system to extract work according to the measurement result. 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 second law of thermodynamics (SLOT).

In the early years after the discovery of the MD, there was insufficient attention to this topic. The first revival of the studies of MD is due to the recognition of the tradeoff between information and entropy in the MD-controlled thermodynamic cycles. The milestone discovery was the "Landauer principle" [4], which reveals that erasing one bit of information from the memory in the computing process inevitably accompanies 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 working substance, and thus erasing the 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 generalization of the Landauer principle, including error effect in the measurement process, has been discussed in Ref. [6].

The recent revival of studies of MD is due to the development of quantum information science. The corresponding quantum thermodynamics concerns quantum heat engines

(QHEs) [7,8] with the quantum coherent system serving as the working substance. The quantum working substance deviates from the thermodynamic limit and preserves its quantum coherence [9,10] to some extent, and thus it has tremendous influence on the properties of QHEs, especially when quantum MD is included in the thermodynamical cycle [11–13]. There have been many attempts to generalize the SHE by quantum mechanically approaching the measurement process [11], the motion control [12], and the insertion and expansion processes [14]. However, to our best knowledge, a fully quantum approach for all processes in the SHE intrinsically integrated with a quantum MD is still lacking. The quantum-classical hybrid description of the SHE may result in some observations about the MD-assisted thermodynamic process that seem to challenge common senses in physics. Therefore, we need a fully quantum theory for MD-assisted thermodynamics.

In this paper, we propose a quantum SHE assisted by MD with a finite temperature difference from that of the system. In this model, we give a consistent quantum approach to the measurement process without using the von Neumann projection [15]. Then we calculate the work done by the insertion of the movable wall in the framework of quantum mechanics. The controlled gas expansion is treated with quantum conditional dynamics. Furthermore, we also consider the process of removing the wall to complete a thermodynamic cycle. With these necessary subtle considerations, the quantum approach for the MD-assisted thermodynamic cycle will go beyond the conventional theories about the SHE. We show that a system that deviates from the thermodynamic limit exhibits uncommon observable quantum effects due to the finite size of system, which results in discrete energy levels that could be washed out by the heat fluctuation. Quantum coherence can assist the MD in extracting more work by reducing effective temperature, while thermal excitation of the MD at a finite temperature would reduce its quantum measurement and conditional control of the expansion. It means that the MD could help the molecule do maximum work outside only when cooled to absolute zero temperature.

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Our paper is organized as follows: In Sec. II we first give a brief review of the classical version of SHE and then present our model in a quantum version with MD included intrinsically. The role of quantum coherence of MD is emphasized with the definition of the effective temperature for an arbitrary two-level system. In Sec. III, we consider the quantum SHE with a quantum MD at finite temperature, measuring the molecular position in a one-dimensional infinitely deep well. The whole cycle consists of four steps: insertion, measurement, expansion, and removal. Detailed descriptions are given subsequently. We calculate the work done and heat exchange in every 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 first revisit Szilard's single-molecule heat engine in brief. As illustrated in Fig. 1(a), the whole thermodynamic cycle consists of three steps: insertion [(i) and (ii)], measurement [(ii) and (iii)], and controlled expansion [(iii) and (iv)] by the MD. The outside agent first 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. Without losing generality, we label the initial state of the demon as 0. Finding that the molecule is on the right, namely $L/2 < x < L$, the demon changes its own memory to state 1, but 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 confining the single molecule: It allows the isothermal expansion with the piston moving from $L/2$ to L if its memory registers 0 and allows the expansion with the piston moving from $L/2$ to 0 if the register is on state 1. In each thermodynamic cycle, the system does work $W = k_B T \ln 2$ to the outside agent in the isothermal expansion. Overall, the system extracts heat from a single heat bath to do work and thus it would violate the SLOT if the MD were not treated as a part of the working substance in the SHE. However, after the cycle, MD stores one-bit information as its final state and is on the mixture state of 0 and 1 with equal probability. Thus, it does not return to its initial state 0. Landauer's principle states that to erase such a bit of information at temperature T requires the dissipation of energy of at least $k_B T \ln 2$. The work extracted by the system compensates for the energy of erasing the memory. Therefore, the SLOT is saved. In this sense, the classical version of MD paradox is only a misunderstanding due to ignoring the erasure of the memories of the MD [5].

In most previous investigations about the MD paradox, it is usually assumed that the system and the MD possess the same heat bath. Thus, the whole working substance formed by the system plus the MD would be in equilibrium, and no quantum coherence would exist. 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 is smaller than $k_B T \ln 2$ [12]. Under this circumstance,

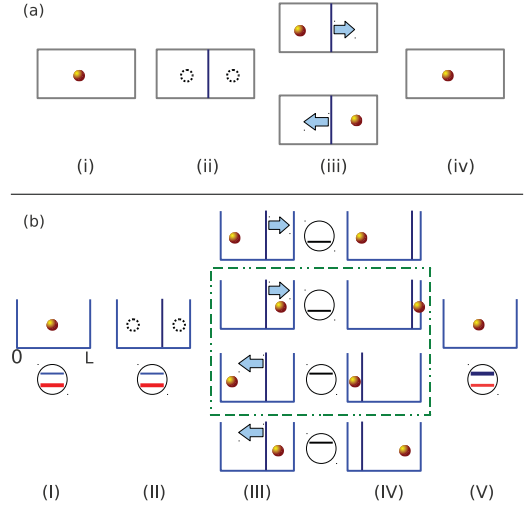


FIG. 1. (Color online) Classical and quantum Szilard's single-molecule heat engine. (a) Classical version: (i), (ii) A piston is inserted in the center of a chamber. (ii), (iii) The demon finds which domain the single molecule stays in. (iii), (iv) The demon controls the system to do work according to 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 an arbitrary position in the potential. (II), (III) The demon measures the state of the system and then records the results in its memory by flipping its own state or not taking action. The measurement may result in the wrong results, illustrated in the green dot-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.

we actually construct a QHE with a nonequilibrium working substance or an equilibrium working substance between two different heat baths. Furthermore, when the MD is initially prepared with quantum coherence, the quantum nature of the whole working substance will result in many exotic features.

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). 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 a thermal state with inverse temperature β . The demon has been in contact with the low-temperature bath at the inverse temperature β_D . The demon is initially prepared in the equilibrium state

$$\rho_0^D = p_g |g\rangle \langle g| + p_e |e\rangle \langle e|, \quad (1)$$

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

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

Actually, the inverse temperature β_D could represent an effective inverse temperature of the MD with quantum coherence. For an environment such as a mesoscopic system, the number of its degrees of freedom is not large. Under this circumstance, the strong coupling to the MD leaves finite off-diagonal elements in the reduced density matrix [16]. This remnant of coherence can be utilized to improve the

apparent efficiency of the heat engine [9,10]. For the demon with coherence, the density matrix usually reads as

$$\rho_0^D = \begin{bmatrix} p_g & F \\ F^* & p_e \end{bmatrix}, \quad (2)$$

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

$$p_+(F) \simeq p_e - \coth\left(\frac{\Delta}{2}\beta_D\right) |F|^2, \quad (3)$$

$$p_-(F) \simeq p_g + \coth\left(\frac{\Delta}{2}\beta_D\right) |F|^2.$$

We can define an effective inverse temperature $\beta_{\text{eff}} = -\ln[p_+(F)/p_-(F)]/\Delta$ 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 in what follows, it is the lowering of the effective temperature of the MD that results in an increase of the heat engine efficiency.

Modeling 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 eigenenergies $E_n(L) = (\hbar n \pi)^2 / (2mL^2)$, where the quantum number n ranges from 1 to ∞ . The initial Hamiltonian can be written as $H_0 = \sum_n E_n(L) |\psi_n(L)\rangle \langle \psi_n(L)|$.

On this set of 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.

With the above model, the MD-assisted thermodynamic cycle for the quantum SHE is divided into the four steps illustrated in Fig. 1(b): (I), (II) the insertion of a mobile solid wall 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 between its two internal states and the spatial wave functions of the confined molecule; (III), (IV) quantum control of the mobile wall to move the according to the record in the demon's memory; and (IV-V) the removal of the wall so that the next thermodynamic cycle can be started. Their descriptions are discussed in the next section.

III. QUANTUM THERMODYNAMIC CYCLES WITH MEASUREMENT

In this section, we analyze in detail 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 may possess a temperature $T_D = 1/\beta_D$ lower than $T = 1/\beta$ of the confined molecule's heat bath. In each step, we evaluate the work done by the outside agent and the heat exchange in detail. In order to concentrate on the physical properties, we put the calculations in Appendix A.

A. Step 1: Quantum insertion [(I) and (II)]

In the first process, the system is in contact with the heat bath β , and 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 lengths 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 eigenvalues $E_n(L-l)$ and $E_n(l)$. In the following discussions, we use the free Hamiltonian $H_T = H + H_D$, where

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

for $0 \leq l \leq L$ and $H_D = \Delta |e\rangle \langle e|$. Here, we take the MD's 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 change. With respect to the above split 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 domains 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 of finding the single molecule on the left and the right sides, 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

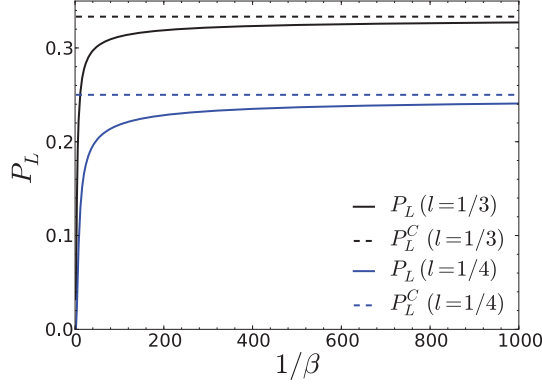


FIG. 2. (Color online) Probability P_L and the corresponding classical one P_L^C vs temperature $1/\beta$ for different piston positions $l = 1/3$ and $l = 1/4$. Without losing generality, we set the parameters as $L = 1$, $m = \pi^2/2$, and $\hbar = 1$.

are different from the classical probabilities, $P_L^c = l/L$ and $P_R^c = (L-l)/L$, of finding the single molecule on the left and right sides. We numerically illustrate this discrepancy between this classical result and ours in Fig. 2 for different insertion positions $l = 1/3$ and $l = 1/4$. It is clear in Fig. 2 that the probability P_L approaches the corresponding classical one P_L^c as the temperature increases to the high-temperature limit. However, a large discrepancy is observed at low temperature. This deviation 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 diminishes with $L \rightarrow \infty$. In this case, the heat excitation will erase 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

$$\Delta U_{\text{ins}} = \text{Tr}[\rho_{\text{ins}} H_T - \rho_0 (H_0 + H_D)]$$

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 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. [14]. By taking 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, one needs the maximum work to be done. Another reasonable fact is that no work is needed to insert the piston at positions $l = 0$ and $l = L$. Classically, it is well known that no work should be done to insert the piston at any position. The classical limit for partition function means that $L \gg \lambda$, where $\lambda = h/\sqrt{2\pi m k_B T}$ is the mean thermal wavelength. However, for a fixed L , it follows the numerical calculation that W_{ins}

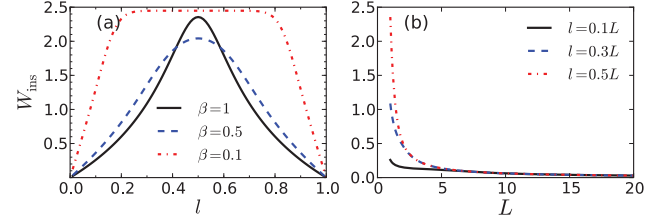


FIG. 3. (Color online) Work done by the outside agent. (a) W_{ins} vs l for different system inverse temperatures $\beta = 1, 0.5$, and 0.1 . Here, we choose the same parameter as in Fig. 2. (b) W_{ins} vs L for different insertion positions $l = 0.1L, 0.3L$, and $0.5L$ with $\beta = 1$.

diverges when the temperature approaches infinity, namely,

$$\lim_{T \rightarrow \infty} W_{\text{ins}} = \infty. \quad (13)$$

This conclusion is mathematically strictly proved in Appendix B. This is different from the conclusion $\lim_{T \rightarrow \infty} W_{\text{ins}} = 0$ obtained in Ref. [14], which can be directly obtained from the result in Eq. (5) in Ref. [11] with $d = 0$. Actually, in Ref. [11], Zurek took the high-temperature limit at the beginning of the calculation of partition function and obtained the result as $k_B T \ln [L/(L-d)]$. We should remark that the final result $k_B T \ln 2$ in both Refs. [11] and [14] is correct since the infinity in whole cycle could be canceled with each other. To explain this inconsistency, we notice that $\lim_{T \rightarrow \infty} \ln [Z(L)/Z(l)] = \ln [L/(L-d)]$. We have $\lim_{d \rightarrow 0} \ln [L/(L-d)] = \lim_{d \rightarrow 0} \lim_{T \rightarrow \infty} \ln [Z_b/Z_{\text{ins}}] = 0$, while $\lim_{T \rightarrow \infty} k_B T = \infty$. Thus, the limit $\lim_{T \rightarrow \infty} W_{\text{ins}} = 0$ cannot be determined with the approximate formula $\ln [L/(L-d)]$. This is similar to the generic problem: Knowing $\lim_{x \rightarrow \infty} f(x) = 0$ and $\lim_{x \rightarrow \infty} g(x) = \infty$, one could not simply determine $\lim_{x \rightarrow \infty} f(x)g(x) = 0$ or ∞ according to some approximation. The right answer depends on the mathematical details rather than some qualitative argument.

The discrete property of the system due to the finite width of the potential well results in a typical quantum effect, even at a high temperature. We can understand this divergence by some consideration in physics. The work W_{ins} to insert a wall is proportional to two factors: the probability of finding a single molecule at the insertion position and the energy of the single molecule. Taking insertion position, $L/2$ for example, the probability decreases as temperature increases and finally reaches a stable with a single molecule staying anywhere in the potential at equal probability $1/L$. However, the average energy for the single molecule keeps increasing. This results in a divergence of W_{ins} for high temperature. This finite-size-induced quantum effect is typical for a 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

$$\lim_{L \rightarrow \infty} W_{\text{ins}} = 0, \quad (14)$$

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

After the insertion of the 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

$$Q_{\text{ins}} = \left(T - \frac{\partial}{\partial \beta} \right) [\ln Z(L) - \ln Z(l)]. \quad (15)$$

Similar to the asymptotic properties of the work in Eq. (14), Q_{ins} approaches to zero when $L \rightarrow \infty$.

B. Step 2: Quantum measurement [(II) and (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 containing a single molecule. The classical states of the single molecule on the right and left sides are denoted as the states 0 and 1. The memory is designed always as two bistable states with no energy difference $\Delta = 0$, and no energy is needed in the measurement process. This setup based on the ‘‘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 [12]. If the molecule is on the left side, no operation is done, whereas the demon flips its state when finding the molecule on the right. This operation is realized by the following unitary operator:

$$U = \sum_n |\psi_n^L(l)\rangle \langle \psi_n^L(l)| \otimes (|g\rangle \langle g| + |e\rangle \langle e|) + |\psi_n^R(L-l)\rangle \langle \psi_n^R(L-l)| \otimes (|e\rangle \langle g| + \text{H.c.}). \quad (16)$$

We remark that the operation is unitary [17], which is different from the previous discussion [6] of MD with the positive operator valued measure (POVM). 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 the measurement is

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

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,

$$\rho_{\text{mea}} = P_L \rho^L(l) \otimes |g\rangle \langle g| + P_R \rho^R(L-l) \otimes |e\rangle \langle e|. \quad (18)$$

Then the demon can distinguish exactly the domain where the single molecule stays, for example, state $|g\rangle$ representing the molecule on left side and vice versa. At a finite temperature, this correlation gets ambiguous. As illustrated in the dot-dashed green box in Fig. 1(b), the demon actually gets the wrong information about the which domain the molecule stays in. 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. Quantitatively,

this information can be expressed in the form of mutual information [18]:

$$I = p_e \ln p_e + p_g \ln p_g - (P_L p_g + P_R p_e) \ln (P_L p_g + P_R p_e) - (P_L p_e + P_R p_g) \ln (P_L p_e + P_R p_g).$$

For the case $T_D = 0$, we have maximum mutual information $I_{\text{eff}} = -(P_L \ln P_L + P_R \ln P_R)$, while it reaches minimum $I_{\text{min}} = 0$ with $\Delta = 0$.

The worst case is that when we first let the MD become degenerate, that is, $\Delta = 0$, the temperature approaches 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

$$\rho_{\text{mea}} = \frac{1}{2} [\rho^L(l) + \rho^R(L-l)] \otimes \rho_0^D(\Delta = 0). \quad (19)$$

Thus, no information is obtained by the MD. There exists another limiting process that the nondegenerate MD is first prepared in the zero-temperature environment, and then Δ approaches zero. Thus, the state of the MD is on state $|g\rangle \langle g|$. In this case, we get a more accurate MD, as mentioned above. The physical essence of the difference between the two limit processes is in the symmetry breaking [19] (we discuss this again later). With such symmetry breaking, the degenerate MD could also make an ideal measurement. An intuitive understanding for the zero-temperature MD helping to do work is that a more calm MD can see the states of the molecule were clearly and control the molecule more effectively.

Next, we calculate the work done in the measurement process by assuming that the total system is 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 which domain the single molecule stays in, state $|g\rangle$ representing molecule on the left and vice versa. As discussed as follows, the work done by the outside agent here is the main factor to slow 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. It is clear that less work is needed if the insertion position is closer to the right boundary of the potential. The work needed in the measurement process approaches 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.

C. Step 3: Controlled expansion [(III) and (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 and the single molecule performs work to the outside. However, the agent pays some work to move the piston to the right if the MD's memory is inaccurate, for example, the situation in the green dot-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 prove later that the total work extracted is independent of the expansion position chosen here. After the expansion process, the density matrix of the whole system is expressed as

$$\rho_{\text{exp}} = [P_L p_g \rho^L(l_g) + P_R p_e \rho^R(L - l_g)] \otimes |g\rangle\langle g| + [P_L p_e \rho^L(l_e) + P_R p_g \rho^R(L - l_e)] \otimes |e\rangle\langle e|. \quad (20)$$

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

$$W_{\text{exp}} = T[\ln \mathcal{Z}(l) + P_L \ln P_L + P_R \ln P_R - P_L p_g \ln Z(l_g) - P_R p_e \ln Z(L - l_g) - P_L p_e \ln Z(l_e) - P_R p_g \ln Z(L - l_e)]. \quad (21)$$

For a perfect correlation ($p_g = 1$), with the piston moved to the side of the potential, namely $l_g = L$ and $l_e = 0$, 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 that can be extracted in this process. In the classical limit $L \rightarrow \infty$, 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

$$Q_{\text{exp}} = P_L \left(T - \frac{\partial}{\partial \beta} \right) [\ln Z(l) - p_g \ln Z(l_g) - p_e \ln Z(L - l_e)] + P_R \left(T - \frac{\partial}{\partial \beta} \right) [\ln Z(L - l) - p_e \ln Z(L - l_g) - p_g \ln Z(l_e)]. \quad (22)$$

D. Step 4: Removal [(IV) and (V)]

To complete the thermodynamic cycle, the system and the MD should be reset to their own initial states. 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 the piston. However, in an arbitrary process, we can show the importance of removing the piston in the whole cycle. During this process, the system keeps contact with the heat bath with inverse temperature β and the removal is performed isothermally. The density matrix of the total system after removing the piston reads

$$\rho_{\text{rev}} = \sum_n \frac{e^{-\beta E_n(L)}}{Z(L)} |\psi_n(L)\rangle\langle\psi_n(L)| \otimes [(P_L p_g + P_R p_e)|g\rangle\langle g| + (P_L p_e + P_R p_g)|e\rangle\langle e|]. \quad (23)$$

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

$$W_{\text{rev}} = \text{Tr}[\rho_{\text{rev}}(H + H_D) - \rho_{\text{exp}} H_T] - T \text{Tr}[-\rho_{\text{rev}} \ln \rho_{\text{rev}}] + T \text{Tr}[-\rho_{\text{exp}} \ln \rho_{\text{exp}}] \quad (24)$$

and

$$Q_{\text{rev}} = -T \text{Tr}[-\rho_{\text{rev}} \ln \rho_{\text{rev}}] + T \text{Tr}[-\rho_{\text{exp}} \ln \rho_{\text{exp}}], \quad (25)$$

respectively. We refer to Appendix A for the exact expression of those two formulas. The MD now is no longer entangled with the system, and the density matrix of the demon is factorized out as

$$\rho_{\text{rev}}^D = (P_L p_g + P_R p_e)|g\rangle\langle g| + (P_L p_e + P_R p_g)|e\rangle\langle e|. \quad (26)$$

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

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

According to Landauer's principle, 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 do not violate the SLOT, since the whole system functionalizes as a heat engine working between a high-temperature bath and a 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 the environment where the information is erased. In the previous studies, people always set the same temperature for the system and the MD. Thus, the exact mechanism of MD was not clear to a certain extent, especially for SHE. Let us 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.

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

$$P_L p_e + P_R p_g \geq p_e, \quad (27)$$

the MD releases energy into its heat bath. We do not discuss this thermalization process here in detail. 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 the quantum version of the SHE, the quantum coherent based on the finite size of the chamber results in different properties from the classical one. Work is required during the insertion and removal processes, while the same process can be done freely in the classical version. The microscopic model here relates the efficiency of the measurement carried out by the 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,

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

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) [8]. To evaluate the efficiency of QHE, we need to obtain the heat absorbed from the high-temperature heat bath. In contrast to the classical one, the exchange of heat with the high-temperature source persists in each step. The total heat absorbed from the high-temperature source is the sum over all four steps,

$$\begin{aligned} Q_{\text{tot}} &= -(Q_{\text{ins}} + Q_{\text{mea}} + Q_{\text{exp}} + Q_{\text{rev}}) \\ &= T[(p_e \ln p_e + p_g \ln p_g) \\ &\quad - (P_L p_g + P_R p_e) \ln(P_L p_g + P_R p_e) \\ &\quad - (P_L p_e + P_R p_g) \ln(P_L p_e + P_R p_g)]. \end{aligned} \quad (29)$$

It is obviously that $Q_{\text{tot}} = TI$. 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 determine the efficiency of this heat engine in a cycle,

$$\eta = 1 - \frac{P_R(p_g - p_e)\Delta}{Q_{\text{tot}}}. \quad (30)$$

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 those of the classical one, namely $P_L = P_R = 1/2$. The total work extracted here can be written in a simple form,

$$W_{\text{tot}} = T(\ln 2 + p_e \ln p_e + p_g \ln p_g) - (p_g - p_e)\Delta/2. \quad (31)$$

In this special case, to make the system capable of doing work to the outside, there is a requirement for 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 the Carnot heat engine, $\beta_D > 1$. The efficiency of this heat engine reads

$$\eta = 1 - \frac{(p_g - p_e)\Delta}{2T(\ln 2 + p_e \ln p_e + p_g \ln p_g)}, \quad (32)$$

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 the efficiency of the heat engine versus the position of the wall l and the temperature of demon β_D in Figs. 4 and 5. As illustrated in Fig. 4(c), for small insertion positions, for example, $l = 0.16$ and 0.36 , the system cannot extract positive work. There exists a critical insertion position l_{cri} to extract positive work, namely,

$$T(P_L^{\text{cri}} \ln P_L^{\text{cri}} + P_R^{\text{cri}} \ln P_R^{\text{cri}}) + P_R^{\text{cri}} \Delta = 0, \quad (33)$$

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 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 Figs. 4(b) and 4(c). Since the high-energy

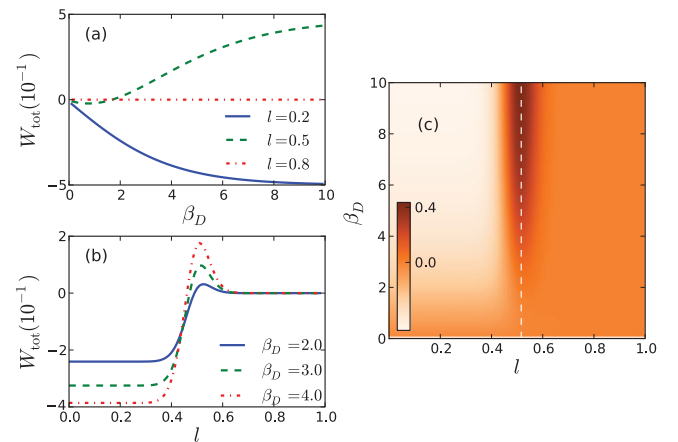


FIG. 4. (Color online) Work vs insertion position l and MD's inverse temperature β_D . (a) Total work as a function of β_D for $l = 0.2$, 0.5 , and 0.8 . (b) Total work as a function of insertion position l for $\beta_D = 2.0$, 3.0 , and 4.0 . (c) Contour plot for total work as function of l and β_D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

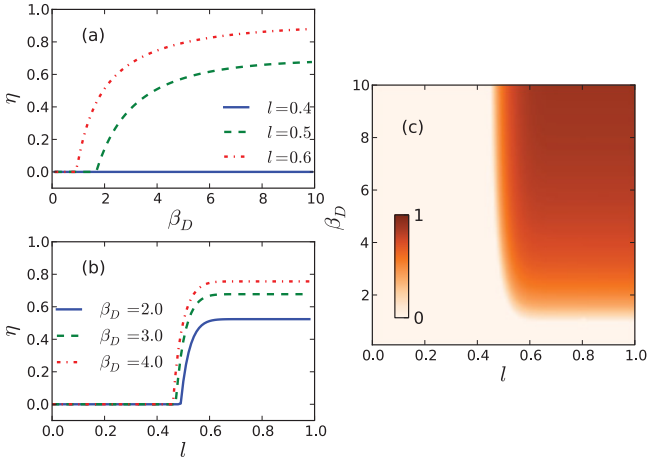


FIG. 5. (Color online) Efficiency vs insertion position l and inverse temperature β_D . (a) Efficiency as a function of β_D for $l = 0.4, 0.5,$ and 0.6 . (b) Efficiency as a function l for $\beta_D = 2, 3,$ and 4 . (c) Contour plot of efficiency vs l and β_D .

state $|e\rangle$ of the demon is utilized to register the right side for a single molecule, more work is need when $l < L/2$. Due to the requirement of work done by the 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 when

$$\frac{P_L^{\text{wmax}} p_e + P_R^{\text{wmax}} p_g}{P_L^{\text{wmax}} p_g + P_R^{\text{wmax}} p_e} = e^{-\beta\Delta}, \quad (34)$$

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-molecule heat engine. We consider only the positive work situation and set efficiency as 0 for all the negative work area. Figure 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 Figs. 5(b) and 5(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 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 attention to two limit processes [19]:

$$\lim_{\beta_D \rightarrow +\infty} \lim_{\Delta \rightarrow 0} \rho_D = (|g\rangle \langle g| + |e\rangle \langle e|) / 2, \quad (35)$$

$$\lim_{\Delta \rightarrow 0} \lim_{\beta_D \rightarrow +\infty} \rho_D = |g\rangle \langle g|. \quad (36)$$

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 different work extracted, namely,

$$\lim_{\beta_D \rightarrow +\infty} \lim_{\Delta \rightarrow 0} W_{\text{tot}} = 0, \quad (37)$$

$$\lim_{\Delta \rightarrow 0} \lim_{\beta_D \rightarrow +\infty} W_{\text{tot}} = k_B T \ln 2. \quad (38)$$

The former one means that MD actually gets no information about the position of the molecule and extracts no work, while the latter one shows 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 [19].

V. CONCLUSIONS

In summary, we have studied a quantum version of SHE with a quantum MD at a finite temperature lower than that of the system. Overall, we simplify the MD as a two-level system, which carries out the measurement in quantum fashion and controls the system to do work to the outside agent. In this sense, the MD-assisted thermodynamic cycle is divided into four steps: insertion, measurement, expansion, and removal, 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 the 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 the Carnot heat engine. It is found the efficiency is always less than that of the Carnot heat engine, since the quantum MD is included as the a part of the the whole working 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 are discovered in the quantum thermodynamic cycles: (1) The finite-size effect of the potential well is found as the reason for the nonvanishing work required in the insertion and removal of the middle wall, 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. (4) In the whole thermodynamic cycle, the removing process is necessary in returning to the initial state for the whole working substance. This fact is neglected in 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 comprehensive understanding about some fundamental

problems in thermodynamics, such as the relationship between quantum unitarity and SLOT [20]. Also, the nonequilibrium properties related to Jarzynski and Crooks's theorem [21] can be discussed in this model.

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APPENDIX A: DETAILED CALCULATION IN EACH STEP

In this appendix, we present a detailed calculation for the work done and efficiency of SHE. Following the calculations for the four steps, 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 $\Delta U_{\text{int}} = \text{Tr}[\rho_{\text{ins}} H_T - \rho_0 (H_0 + H_D)]$ and total entropy $\Delta S_{\text{ins}} = \text{Tr}[-\rho_{\text{ins}} \ln \rho_{\text{ins}}] - \text{Tr}[-\rho_0 \ln(\rho_0)]$ are explicitly given by

$$\Delta U_{\text{int}} = \sum_n p_n(l) E_n(l) + \sum_n p_n(L') E_n(L') - \sum_n p_n(L) E_n(L) = \frac{\partial}{\partial \beta} [\ln Z(L) - \ln Z(l)], \quad (\text{A1})$$

where $L' = L - l$ and

$$\Delta S_{\text{ins}} = [\ln Z(l) - \ln Z(L)] + \beta \sum_n \left[\frac{p_n(l) E_n(l)}{+p_n(L') E_n(L')} - p_n(L) E_n(L) \right] = \left(1 - \beta \frac{\partial}{\partial \beta} \right) [\ln Z(l) - \ln Z(L)], \quad (\text{A2})$$

where

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

For the isothermal process, the work done by the 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,

$$W_{\text{ins}} = T [\ln Z(L) - \ln Z(l)], \quad (\text{A3})$$

$$Q_{\text{ins}} = \left(T - \frac{\partial}{\partial \beta} \right) [\ln Z(L) - \ln Z(l)]. \quad (\text{A4})$$

Step 2: Measurement. The measurement is realized by a controlled-NOT unitary operation, which has been illustrated clearly in Sec. II. After the measurement process, the density matrix for the total system is

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

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

$$W_{\text{mea}} = \Delta U_{\text{mea}} = P_R(p_g - p_e)\Delta. \quad (\text{A5})$$

Step 3: Controlled expansion. At the ending of expansion, the state for the total system reads

$$\rho_{\text{exp}} = [P_L p_g \rho^L(l_g) + P_R p_e \rho^R(L_g)] \otimes |g\rangle \langle g| + [P_L p_e \rho^L(L_e) + P_R p_g \rho^R(l_e)] \otimes |e\rangle \langle e|.$$

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

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

$$\begin{aligned} W_{\text{exp}} &= \text{Tr}[\rho_{\text{exp}}(H + H_D)] - \text{Tr}[\rho_{\text{mea}}(H + H_D)] - T \text{Tr}[-\rho_{\text{exp}} \ln \rho_{\text{exp}}] + T \text{Tr}[-\rho_{\text{mea}} \ln \rho_{\text{mea}}] \\ &= \sum_n [P_L p_g p_n(l_g) E_n(l_g) + P_R p_e p_n(L_g) E_n(L_g) + P_L p_e p_n(L_e) E_n(L_e) + P_R p_g p_n(l_e) E_n(l_e)] + (P_L p_e + P_R p_g) \Delta \\ &\quad - \left[\sum_n (P_L p_n(l) E_n(l) + P_R p_n(L') E_n(L')) + (P_L p_e + P_R p_g) \Delta \right] + T \sum_n [P_L p_g p_n(l_g) \ln P_L p_g p_n(l_g) \\ &\quad + P_R p_e p_n(L_g) \ln P_R p_e p_n(L_g) + P_L p_e p_n(L_e) \ln P_L p_e p_n(L_e) + P_R p_g p_n(l_e) \ln P_R p_g p_n(l_e)] \\ &\quad - T \sum_n [P_L p_g p_n(l) \ln P_L p_g p_n(l) + P_R p_e p_n(L') \ln P_R p_e p_n(L')] \\ &\quad + P_L p_e p_n(l) \ln P_L p_e p_n(l) + P_R p_g p_n(L') \ln P_R p_g p_n(L')] \end{aligned} \quad (\text{A6})$$

$$= P_L T [\ln Z(l) - p_g \ln Z(l_g) - p_e \ln Z(L_e)] + P_R T [\ln Z(L') - p_e \ln Z(L_g) - p_g \ln Z(l_e)]. \quad (\text{A7})$$

The internal energy changes can be also evaluated as

$$\begin{aligned}
\Delta U_{\text{exp}} &= \sum_n [P_L p_g p_n(l_g) E_n(l_g) + P_R p_e p_n(L_g) E_n(L_g) + P_L p_e p_n(L_e) E_n(L_e) + P_R p_g p_n(l_e) E_n(l_e)] + (P_L p_e + P_R p_g) \Delta \\
&\quad - \left[\sum_n (P_L p_n(l) E_n(l) + P_R p_n(L') E_n(L')) + (P_L p_e + P_R p_g) \Delta \right] \\
&= \sum_n [P_L p_g p_n(l_g) E_n(l_g) + P_R p_e p_n(L_g) E_n(L_g) + P_L p_e p_n(L_e) E_n(L_e) + P_R p_g p_n(l_e) E_n(l_e)] \\
&\quad - \sum_n [P_L p_n(l) E_n(l) + P_R p_n(L') E_n(L')] \\
&= P_L \frac{\partial}{\partial \beta} [\ln Z(l) - p_g \ln Z(l_g) - p_e \ln Z(L_e)] + P_R \frac{\partial}{\partial \beta} [\ln Z(L') - p_e \ln Z(L_g) - p_g \ln Z(l_e)]. \tag{A8}
\end{aligned}$$

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

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

Step 4: Removal. The piston is removed in this process. After that, the system returns to its initial state and is not entangled with MD. The last step would be to remove the wall in the trap. The system is on the state as

$$\rho_{\text{rev}} = \sum_n \frac{\exp[-\beta E_n(L)]}{Z(L)} |\psi_n(L)\rangle \langle \psi_n(L)| \otimes [(P_L p_g + P_R p_e) |g\rangle \langle g| + (P_L p_e + P_R p_g) |e\rangle \langle e|]. \tag{A9}$$

Then, the work done and the heat absorbed are respectively

$$W_{\text{rev}} = \text{Tr}[\rho_{\text{rev}}(H + H_D)] - \text{Tr}[\rho_{\text{exp}}(H + H_D)] - T \text{Tr}[-\rho_{\text{rev}} \ln \rho_{\text{rev}}] + T \text{Tr}[-\rho_{\text{exp}} \ln \rho_{\text{exp}}] \tag{A10}$$

or

$$\begin{aligned}
W_{\text{rev}} &= \sum_n p_n(L) E_n(L) + (P_L p_e + P_R p_g) \Delta \\
&\quad - \sum_n [P_L p_g p_n(l_g) E_n(l_g) + P_R p_e p_n(L_g) E_n(L_g) + P_L p_e p_n(L_e) E_n(L_e) + P_R p_g p_n(l_e) E_n(l_e)] - (P_L p_e + P_R p_g) \Delta \\
&\quad + T \left[\sum_n p_n(L) \ln p_n(L) + (P_L p_g + P_R p_e) \ln(P_L p_g + P_R p_e) + (P_L p_e + P_R p_g) \ln(P_L p_e + P_R p_g) \right] \\
&\quad - T \sum_n \{ P_L p_g p_n(l_g) \ln[P_L p_g p_n(l_g)] + P_R p_e p_n(L_g) \ln[P_R p_e p_n(L_g)] + P_L p_e p_n(L_e) \ln[P_L p_e p_n(L_e)] \\
&\quad + P_R p_g p_n(l_e) \ln[P_R p_g p_n(l_e)] \} \\
&= T \{ -\ln Z(L) + (P_L p_g + P_R p_e) \ln(P_L p_g + P_R p_e) + (P_L p_e + P_R p_g) \ln(P_L p_e + P_R p_g) - P_L \ln P_L - P_R \ln P_R \\
&\quad - p_e \ln p_e - p_g \ln p_g + P_L p_g \ln Z(l_g) + P_R p_e \ln Z(L_g) + P_L p_e \ln Z(L_e) + P_R p_g \ln Z(l_e) \} \tag{A11}
\end{aligned}$$

and

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

$$\begin{aligned}
 &= T[(P_L p_g + P_R p_e) \ln(P_L p_g + P_R p_e) + (P_L p_e + P_R p_g) \ln(P_L p_e + P_R p_g) - P_L \ln P_L - P_R \ln P_R - p_e \ln p_e - p_g \ln p_g] \\
 &\quad - \left(T - \frac{\partial}{\partial \beta}\right) \ln Z(L) + P_L p_g \left(T - \frac{\partial}{\partial \beta}\right) \ln Z(l_g) + P_R p_e \left(T - \frac{\partial}{\partial \beta}\right) \ln Z(L_g) \\
 &\quad + P_L p_e \left(T - \frac{\partial}{\partial \beta}\right) \ln Z(L_e) + P_R p_g \left(T - \frac{\partial}{\partial \beta}\right) \ln Z(l_e). \tag{A12}
 \end{aligned}$$

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

$$\begin{aligned}
 W_{\text{tot}} &= -(W_{\text{ins}} + W_{\text{mea}} + W_{\text{exp}} + W_{\text{rev}}) = T[(p_e \ln p_e + p_g \ln p_g) - (P_L p_g + P_R p_e) \ln(P_L p_g + P_R p_e) \\
 &\quad - (P_L p_e + P_R p_g) \ln(P_L p_e + P_R p_g)] - P_R(p_g - p_e)\Delta. \tag{A13}
 \end{aligned}$$

The total heat absorbed can also be obtained as

$$Q_{\text{tot}} = -(Q_{\text{ins}} + Q_{\text{exp}} + Q_{\text{rev}}) = T \left[\begin{aligned} &(p_e \ln p_e + p_g \ln p_g) - (P_L p_g + P_R p_e) \ln(P_L p_g + P_R p_e) \\ &- (P_L p_e + P_R p_g) \ln(P_L p_e + P_R p_g) \end{aligned} \right]. \tag{A14}$$

APPENDIX B: PROOF OF THE LIMITATION

In this appendix, we mathematically consider the limit behavior of the insertion work

$$W_{\text{ins}}(\beta) = \frac{1}{\beta} \ln \frac{\sum_{n=1}^{\infty} \exp(-\beta n^2 \alpha^2 / L^2)}{2 \sum_{n=1}^{\infty} \exp(-4\beta n^2 \alpha^2 / L^2)} \tag{B1}$$

as $\beta \rightarrow 0$. To this end, we first estimate the series

$$S(k) \equiv \sum_{n=1}^{\infty} e^{-kn^2}, \tag{B2}$$

where k is a positive real number. Actually, we can approximate the series $S(k)$ with integrals of $f(x) = \exp(-kx^2)$ over two domains $(1, \infty)$ and $(0, \infty)$ respectively. After re-expressing the two integrals back to two sums approximately in Figs. 6(a) and 6(b), we observe

$$\int_1^{\infty} e^{-kx^2} dx < \sum_{n=1}^{\infty} e^{-kn^2} < \int_0^{\infty} e^{-kx^2} dx.$$

When we noticed that $\int_0^{\infty} \exp(-kx^2) dx = \sqrt{\pi/(4k)}$, it is easy to prove that the deviation

$$\begin{aligned}
 c(k) &\equiv \int_0^{\infty} e^{-kx^2} dx - \sum_{n=1}^{\infty} e^{-kn^2} \\
 &= \sqrt{\frac{\pi}{4k}} - S(k) \tag{B3}
 \end{aligned}$$

satisfies

$$0 < c(k) < \int_0^1 e^{-kx^2} dx < \int_0^1 dx = 1. \tag{B4}$$

This estimate about the bound of $c(k)$ is coarse for practice, but a more precise estimate shows that

$$\lim_{k \rightarrow 0} c(k) = \frac{1}{2}. \tag{B5}$$

The detailed calculation can be found in Appendix. This result could be verified by the numerical simulation. Therefore, we conclude that

$$\lim_{k \rightarrow 0} S(k) \rightarrow \sqrt{\frac{\pi}{4k}} - \frac{1}{2}. \tag{B6}$$

Next, we use the above result in Eq. (B6) to estimate $W_{\text{ins}}(\beta)$. With the above definition, we rewrite $W_{\text{ins}}(\beta)$ as

$$W_{\text{ins}}(\beta) = \frac{1}{\beta} \ln \frac{1 - 2c(z)\sqrt{z/\pi}}{1 - 4c(4z)\sqrt{z/\pi}}, \tag{B7}$$

where $z = \beta\alpha^2/L^2$. Now, let us consider the high-temperature case, in which $c(z)\sqrt{z/\pi}$ and $c(4z)\sqrt{z/\pi}$ are much less than unity. A straightforward calculation gives

$$\begin{aligned}
 W_{\text{ins}} &= \frac{1}{\beta} \ln\{[1 - 2c(z)\sqrt{z/\pi}][1 + 4c(4z)\sqrt{z/\pi} + O(\beta)]\} \\
 &= \frac{1}{\beta} \ln[1 + (4c(4z) - 2c(z))\sqrt{z/\pi} + O(\beta)] \\
 &= \frac{1}{\beta} [(4c(4z) - 2c(z))\sqrt{z/\pi} + O(\beta)] \\
 &= \frac{2a}{\sqrt{\pi}L} \frac{2c(4z) - c(z)}{\sqrt{\beta}} + O(1). \tag{B8}
 \end{aligned}$$

Finally, we mathematically strictly prove our claim that the work for insertion diverges as temperature tends to infinity, namely,

$$\lim_{\beta \rightarrow 0} W_{\text{ins}} = \lim_{\beta \rightarrow 0} \frac{a}{\sqrt{\pi}\beta L} = \infty. \tag{B9}$$

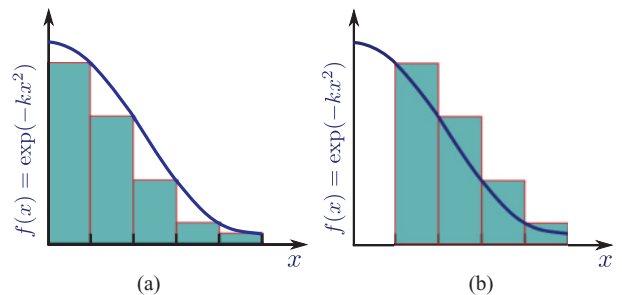


FIG. 6. (Color online) Comparison between summation and integral over two domains (a) $(0, \infty)$ and (b) $(1, \infty)$. The summation is marked as these filled area in both panels.

- [1] H. S. Leff and A. F. Rex, eds., *Maxwell's Demon 2: Entropy, Classical and Quantum Information, Computing* (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. Sagawa and M. Ueda, *Phys. Rev. Lett.* **102**, 250602 (2009).
- [7] T. D. Kieu, *Phys. Rev. Lett.* **93**, 140403 (2004); *Eur. Phys. J. D* **39**, 115 (2006).
- [8] H. T. Quan, Y.-X. Liu, C. P. Sun, and F. Nori, *Phys. Rev. E* **76**, 031105 (2007); H. T. Quan, *ibid.* **79**, 041129 (2009).
- [9] M. O. Scully, M. S. Zubairy, G. S. Agarwal, and H. Walther, *Science* **299**, 862 (2003).
- [10] H. T. Quan, P. Zhang, and C. P. Sun, *Phys. Rev. E* **73**, 036122 (2006).
- [11] W. H. Zurek, in *Proceedings Frontiers of Nonequilibrium Quantum Statistical Mechanics*, edited by G. T. Moore and M. O. Scully (Plenum, 1986), pp. 145–150.
- [12] H. T. Quan, Y. D. Wang, Y.-X. Liu, C. P. Sun, and F. Nori, *Phys. Rev. Lett.* **97**, 180402 (2006).
- [13] S. Lloyd, *Phys. Rev. A* **56**, 3374 (1997).
- [14] S. W. Kim, T. Sagawa, S. DeLiberato, and M. Ueda, *Phys. Rev. Lett.* **106**, 070401 (2011).
- [15] P. Zhang, X. F. Liu, and C. P. Sun, *Phys. Rev. A* **66**, 042104 (2002).
- [16] H. Dong, S. Yang, X. F. Liu, and C. P. Sun, *Phys. Rev. A* **76**, 044104 (2007).
- [17] E. Joos and H. D. Zeh, *Z. Phys. B* **59**, 2231 (1985); R. Omnes, *Rev. Mod. Phys.* **64**, 339 (1992); C. P. Sun, X. X. Yi, and X.-J. Liu, *Fortschr. Phys.* **43**, 7 (1995); W. H. Zurek, *Rev. Mod. Phys.* **75**, 715 (2003).
- [18] T. Sagawa and M. Ueda, *Phys. Rev. Lett.* **100**, 080403 (2008).
- [19] J.-Q. Liao, H. Dong, X. G. Wang, X. F. Liu, and C. P. Sun, e-print arXiv:0909.1230.
- [20] H. Dong, D. Z. Xu, and C. P. Sun (unpublished).
- [21] C. Jarzynski, *Phys. Rev. Lett.* **78**, 2690 (2007); G. E. Crooks, *J. Stat. Phys.* **90**, 1481 (1998); R. Kawai, J. M. R. Parrondo, and C. Van den Broeck, *Phys. Rev. Lett.* **98**, 080602 (2007).