Optimal work of the quantum Szilard engine under isothermal processes with inevitable irreversibility

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Abstract

We have found the optimal conditions for work performed by the quantum Szilard engine (SZE) containing multi-particles under isothermal processes with inevitable irreversibility. We define the restorability as the probability that the reversibility of an engine with inevitable irreversibility is achieved when the time-backward process is performed. The optimal condition is then obtained when the restorability is maximized. This is equivalent to the condition that the time-forward force is equal to that of time-backward force. We numerically confirm our expectation by using the quantum SZE containing three bosons or fermions.

1. Introduction

Maxwell was the first to ask a deep physical question about the nature of information using his famous demon [1]. Szilard then recognized the connection between information and entropy demonstrated by his thought experiment called the Szilard engine (SZE) [2]. It tells us that one can extract work from a cyclic engine with a single heat bath with a single temperature by exploiting information. It seems to violate Carnot’s version of the second law of thermodynamics. However, it is now widely accepted that the SZE does not violate the second law and the Carnot’s principle must be modified [3–5]. The SZE has been realized in various experiments [6–11].

Carnot showed that an optimal engine is achieved when its thermodynamic processes are reversible. For the SZE containing multi-particles, however, it is known that the irreversibility inevitably occurs [12–16]. To optimize the work of a classical multi-particle SZE, Horowitz and Parrondo have proposed an extremely sophisticated protocol to make the feedback process reversible [14]. On the other hand, achievable bounds of extractable work [15], non-equilibrium equalities [16], and its quantum version [17] have been found with the irreversibility kept intact. Recently Wehner et al report the relation between the reversibility of quantum thermodynamic processes and the corresponding work [18]. Diaz de la Cruz and Martin-Delgado have studied optimal extractable work of heat engines with many-body states by controlling quantum-information [19]. Cai et al have found the optimal condition of quantum SZE similar to this paper, but they did not seriously consider irreversible case [20].

The main question addressed in this paper is what the optimal condition of extractable work of the quantum SZE is when its inevitable irreversibility [13, 15–17, 21] is taken into account. Due to the irreversibility an initial state at the stage that the inevitably irreversible process occurs cannot be automatically restored when the time-backward process is performed. There exists a certain probability that we return the initial state for time-backward process. We call such a probability the restorability. The similar quantity has been found and interpreted as unavailable information [15, 16]. We show that the optimal work is achieved when the restorability is maximized. This seems to physically make sense considering Carnot’s argument that a reversible engine is optimal. It is also equivalent to the condition that the force of time-forward is equal to that of time-backward (defined below). It has important consequences since the force of time-backward always vanishes in classical mechanics but in general has non-zero value in quantum mechanics. Thus it exhibits difference between classical and quantum mechanics in achieving an optimal engine.
This paper is organized as follows. In section 2, we briefly introduce the thermodynamic processes of quantum SZE and the work formula. In section 3, we discuss physical reasons why irreversibility inevitably occurs in a SZE. In section 4, we find the mathematical condition for optimal work, and discuss its physical meaning. In section 5, we confirm our finding by using a simple example, quantum SZE containing three particles. Finally, in section 6 we summarize our paper.

2. Quantum Szilard engine

There are four stages in the thermodynamic cycle of a SZE containing N particles with temperature T in a closed cylinder of horizontal length L as shown in figure 1. The stages involve (i) inserting a wall in the vertical direction at $l = l(l(0 \leq l \leq L)$, (ii) measuring the number of particles $m$ on the left side, (iii) performing isothermal expansion, where the wall stops at $x = x_m$ differing in $m$, and (iv) removing the wall to complete the cycle. The quantum mechanical work done by the SZE is given by

$$W = -k_B T \sum_{m=0}^{N} f_m(l) \ln \left[ \frac{f_m(l)}{f_m(x_m)} \right]$$

with $f_m(l) = Z_{m}(l)/Z(l)$, $f_m^{\prime}(x_m) = Z_{m}(x_m)/Z(x_m)$ [12]. $k_B$ denotes the Boltzmann constant. Here, $Z_m(l)$ and $Z_m(x_m)$ denotes the partition function of the case where $m$ particles are on the left side of the wall, i.e. $N - m$ particles on the right, when the wall is located at $l$ and $x_m$, respectively, and $Z(l) = \sum_m Z_m(l)$ and $Z(x_m) = \sum_m Z_m(x_m)Z_m(x_m)$. As we consider the quantum SZE, the indistinguishability of the particles should be appropriately taken into account when constructing the partition functions. Note that $l$ is chosen freely when the wall is inserted, while $x_m$ is determined from the force balance, $F^L + F^R = 0$. The force balance position is denoted as $x_m^0$. The force (or pressure) exerted upon the wall by particles along $x$ direction on the left (right) side is defined as

$$F^L(x) = -\sum_n p_n^{L(R)} \left[ \frac{\partial E_n^{L(R)}}{\partial x} \right],$$

where $p_n^{L(R)}$ and $E_n^{L(R)}$ represent the occupation probability and the eigenenergy of the nth energy level of the left (right) side, respectively. Note that we require all thermodynamic processes of the quantum SZE to be isothermal. This guarantees that the temperature of the engine is always kept constant during the whole cycle so that the quantum SZE extracts work from a single heat bath with a single temperature, similar to the classical SZE. The issue of Maxwell’s demon has also been discussed in the quantum SZE [22].

Although (1) is derived for the quantum SZE, surprisingly, it also describes the work of the classical SZE derived from the dissipative work theorem of classical non-equilibrium thermodynamics [13, 21]. The reason why the non-equilibrium thermodynamics comes into play is that removing the wall separating particles into two parts is irreversible. This is nothing but free expansion [23].

Even though both the quantum and classical SZE have equivalent mathematical forms of works, i.e. (1), the partition functions differ, and so does the amount of the work [13]. Note that information itself is inherently
classical here [13]. Recently, a heat engine exploiting purely quantum mechanical information was proposed [24, 25].

3. Inevitable irreversibility

In this section, we explain why irreversibility inevitably takes place in multi-particle SZE in physical point of view. It has been found that the work of (1) at the low-temperature limit can be negative, as shown in figure 2, implying work should be done on the engine rather than extracted from it [26–28]. To clarify what physically happens, let us consider a specific example, a quantum SZE containing three bosons at the low temperature limit, which implies that considering only the lowest energy level is sufficient. We focus on the case where two bosons on the left and one on the right are obtained when the measurement is performed. Isothermal expansion follows such that the wall stops at the position where the force balance condition, \( F^L + F^R = 0 \), is satisfied. It is not optimal and even worse in extracting work to stop the wall at the force balance point [29] originally proposed in [12]. At this time, the right and left sides are completely separated, and the total Hamiltonian \( H \) can be written as \( H = H_L + H_R \), where \( H_{L(R)} \) denotes the Hamiltonian describing only the left (right) side. Then the state of the bosons is described as \( |0\rangle_L |0\rangle_L |0\rangle_R \) with \( H_{L(R)} |n\rangle_{L(R)} = E_{n(L)} |n\rangle_{L(R)} \).

The wall removal is described as a horizontally sliding thin impenetrable barrier, as shown in inset (b) of figure 2. Once the wall just opened so that a tiny gap bridging the left and right sides is formed, the eigenstates previously localized on each side become delocalized over both sides: \( |0\rangle_L \rightarrow |0\rangle \) and \( |0\rangle_R \rightarrow |\tilde{1}\rangle \) with \( \tilde{H} |\tilde{1}\rangle = \tilde{E}_0 |\tilde{1}\rangle \). Here the total Hamiltonian is given as \( \tilde{H} = H_L + H_R + \alpha H_i \), where \( H_i \) denotes the coupling between the left and right side, and \( \alpha \ll 1 \). Note that \( E_1^L \approx E_0^L \) and \( E_0^R \approx \tilde{E}_0 \). The engine is then equilibrated with a thermal heat bath due to the isothermal process, so that the boson at the upper level of the whole engine is quickly relaxed to the ground state; namely \( |1\rangle \rightarrow |0\rangle \), as shown in inset (b) of figure 2. Here, we safely assume such a relaxation takes place fast enough compared with the operational time scale [20].

The transitions occurring are summarized as follows

\[
|0\rangle_L |0\rangle_L |0\rangle_R \xrightarrow{\text{II}} |\tilde{1}\rangle |\tilde{0}\rangle |\tilde{0}\rangle \xrightarrow{\text{II}} |\tilde{0}\rangle |\tilde{0}\rangle |\tilde{0}\rangle ,
\]

where we ignore the symmetrization of bosonic states for simplicity. The transition (II) is irreversible relaxation that gives rise to energy dissipation, which causes negative work. The irreversibility occurring at the wall removal is inevitable in multi-particle quantum SZE.

In a usual heat engine, the optimal conditions of work are achieved when the whole thermodynamic process is reversible. However, in the multi-particle quantum SZE it is unlikely to make the whole thermodynamic process reversible since removing the wall is inevitably irreversible. This raises questions about what the physical meaning is for the optimal conditions of an engine with inevitable irreversibility. The intrinsic singularity resulting from such irreversibility has been investigated in other studies in [11, 15–17, 30]. The optimal conditions of an information heat engine have also been investigated in various contexts [14, 15, 31–34].
4. Optimal condition

Let us now find the mathematical condition for optimal work of the quantum SZE. Equation (1) is a function of \( l \) and \( \{ x_m \} \) with \( m = 0, 1, \ldots, N \), namely \( W ( l, \{ x_m \} ) \). The optimal (maximum) conditions are obtained from \( \partial W / \partial l = 0 \) and \( \partial W / \partial x_m = 0 \).\(^1\) The latter condition is equivalent to

\[
\frac{\partial \ln f_m(x_m)}{\partial x_m} = 0,
\]

which has simple physical interpretation. \( f_m(x_m) \) represents the probability to choose the case of \( m \) particles on the left side of the wall when the wall is inserted at \( x_m \) in time-forward process, where \( x_m \) denotes the position at which the wall stops when \( m \) particles are on the left side in time-forward process. For example, assume we have one boson on the left and start to remove the wall located at \( x_1 \) in time-forward process as shown in figure 3(a). Now let us consider its time-backward process. It is impossible to automatically return to the initial state of time-forward process. Instead we have many possible cases as shown in figure 3(b). There exists a certain probability to return, which is defined as \( f_m(x_m) \). In fact, it is also interpreted as the probability that the reversibility of the engine is restored.

Thus we call it ‘restorability’. We then say that the optimal condition of the quantum SZE is achieved when the restorability is maximized. Note that similar argument has been discussed in \([15]\).

The optimal condition obtained above is equally applicable to both classical and quantum mechanics since the work formula (1) mathematically has equivalent form \([13]\). In \([29]\), however, in the quantum SZE the optimal work is not achieved at the force balance where the classical SZE is optimal. It raises a question on where such difference comes from. To address it we now consider the force. Equation (4) is rewritten as

\[
\frac{1}{Z_m} \frac{\partial Z_m}{\partial x_m} = \frac{1}{Z} \frac{\partial Z}{\partial x_m}
\]

with \( Z(x_m) = \sum_p Z_p(x_m) \). The partition function \( Z_m \) is given as

\[
Z_m(x_m) = \sum_p e^{-\beta \epsilon_m^p(x_m)}
\]

with \( \epsilon_m^p = \sum_n (E_n^L m_n^p + E_n^R q_n^p) \), where \( m_n^p \) and \( q_n^p \) represent the number of particles occupying the \( n \)th energy level of the left and right sides, respectively, satisfying \( m = \sum_n m_n^p \) and \( N - m = \sum_n q_n^p \). Here \( \sigma \) denotes the possible configuration of particles depending on whether they are bosons or fermions over all the energy levels for a given \( m, m_n^p \) and \( q_n^p = 0 \) only either 0 or 1 in fermions while 0, 1, \ldots, \( m \) and 0, 1, \ldots, \( N - m \), respectively, in bosons.

The left-hand side of (5) represents the net force on the wall multiplied by the inverse temperature when \( m \) particles are on the left side due to

\(^1\) In fact, these guarantee that they are only extrema. Instead of finding their second derivatives, we have confirmed they are maxima by directly plotting them like figure 4.
\[ \frac{1}{Z_m} \frac{\partial Z_m}{\partial x_m} = -\beta \left\{ \frac{\partial e_m^L}{\partial x_m} \right\}_o \equiv \beta F_m \]  

(7)

with \( \beta = 1/k_B T \). Note that \( F_m(x_m^o) = 0 \) gives rise to the force balance conditions. The right-hand side of (5) is expressed as

\[ \frac{1}{Z} \frac{\partial Z}{\partial x_m} = \frac{1}{Z} \sum_p \frac{\partial Z_p}{\partial x_m} = -\beta \sum_p \frac{Z_p}{Z} \left\{ \frac{\partial e_p^L}{\partial x_m} \right\}_o \equiv \beta \langle F_p \rangle_p. \]  

(8)

The force \( \langle F_p \rangle_p \) of (8) is obtained from averaging \( F_p \). To understand its physical meaning let us consider the time-forward and time-backward processes of removing the wall in detail. For the time-forward process, the number of particles on the left, \( m \), is determined once the measurement is performed, and then is kept constant before we remove the wall at \( x_m \). For the time-backward process, we cannot automatically go back to the case of \( m \) since the number of particles on the left can be any integer in \([0, N]\) when the wall is inserted at \( x_m \) as shown in figure 3. Thus in some sense \( \langle F_p \rangle_p \) is regarded as the force for the time-backward.

From equations (7) and (8), the optimal conditions (5) can be rewritten as

\[ F_m(x_m^o) = \langle F_p (x_m^o) \rangle_p. \]  

(9)

The optimal \( x_m^o \) is obtained from the conditions where the force of the time-forward process is equivalent to that of the time-backward process. Although, the work obtained from the force balance, \( F_m(x_m^o) = 0 \), can become negative at low temperatures, the work at the optimal condition (9) is always non-negative. The proof is as follows. Mathematically, the form of \( f_m \) is equivalent to that of \( f_m^o \), namely \( f_m(y) = f_m^o(y) \). Since the optimal work is obtained from maximizing \( f_m^o \) (see equation (1)), i.e. \( \partial \ln f_m^o(x_m)/\partial x_m = 0 \), we obtain \( f_m(t) = f_m^o(t) \leq f_m^o(x_m^o) \) irrespective of \( l \). This immediately implies that the work of (1) at the maximum is non-negative.

It is quantum effect that the force balance condition is different from the optimal condition. For classical particles, satisfying ideal gas law for simplicity, one finds

\[ \beta \langle F_p (y) \rangle_p = \sum_{p=0}^N P(p) \left( \frac{p}{y} - \frac{N-p}{L-y} \right) = 0 \]  

for any \( y \in (0, L) \) with

\[ P(p) = \left( \frac{y}{L} \right)^p \left( \frac{L-y}{L} \right)^{N-p} \left( \frac{N}{p} \right). \]  

(11)

The optimal conditions are thus achieved simply by the force balance, since the right-hand side of (9) always vanishes.

The fact that \( \langle F_p (x_m^o) \rangle_p \) does not vanish in quantum mechanics seems weird. The reason is that the non-zero net average force cannot be obtained simply by inserting the wall according to the second law of thermodynamics. If the wall is inserted at \( x = L/2 \), in quantum mechanics the structures of energy levels of the left side become different from those of the right. Thus, the corresponding generalized forces of both sides are not necessarily equivalent, i.e. \( \sum_n \epsilon_n^L \langle \partial E_n^L / \partial x \rangle = \sum_n \epsilon_n^R \langle \partial E_n^R / \partial x \rangle \) from (2). It gives rise to non-zero net force on the wall. Interestingly this seems to be similar to Casimir-like effect as far as only the similarity of their mathematical description is concerned [36–38].

So far, we have discussed the optimal conditions of \( \{x_m\} \). The optimal conditions of \( l \) are rather subtle. Intuitively, one expects the symmetric point \( l = L/2 \) to satisfy the optimal conditions. We can at least show that the work (1) has an extremum at \( l = L/2 \). In general, however, the work does not always exhibit a global maximum at \( l = L/2 \). We set \( x_m = x_m^o \) since \( x_m^o \) has nothing to do with \( l \). From \( \partial W / \partial l = 0 \) we obtain

\[ \langle W_m(l, x_m^o) \rangle = \langle W_p(l, x_p^o) \rangle_p \langle E_p(l) \rangle. \]  

(12)

with \( W_m(l, y) = -\ln \left[ f_m^o(l) f_m^o(y) \right] \). Both the left and right hand sides of (12) vanish at \( l = L/2 \) according to \( f_m^o(L/2) = f_m^o(L/2) \), \( W_m^L(L/2, x_m^o) = W_m^R(L/2, x_m^o) \), and \( F_m^L(L/2) = F_m^R(L/2) \), so that the work exhibits an extremum at \( l = L/2 \). However, this is not a unique extremum. For example, figure 4 shows that a single maximum of the work of an SZE containing two spinless fermions splits into two peaks as temperature decreases, although the work retains an extremum at \( l = L/2 \). This splitting is associated with the accidental degeneracies of the problem and the exclusion principle of fermions [39]. The optimal conditions of the work of \( l \) thus depend on the temperature and the number of particles only in fermions, so that it is not easy to find a simple mathematical expression. However, we set \( l = L/2 \) since it is the optimal condition for fermions except extremely low temperature and for bosons over the whole range of temperature. Moreover, the irreversibility of the SZE is associated with \( x_m \) at which the wall is removed, rather than \( l \), at which the wall is inserted.
5. Example and remark

Now let us consider a quantum SZE containing three particles as an example to confirm our theory. Below, we consider the engine in one-dimension for simplicity. The wall is modeled as a potential barrier with negligibly small width, i.e. a delta-function potential with height $V$. The wall removal is then described as decreasing $V$ from $\infty$ to 0. We assume that the particles are immediately relaxed once the wall is no longer perfect ($x_0 = 0$).

The engine is described by a one-dimensional infinite potential well. We insert the wall at $L/2$ as above. Recall that the optimal work is obtained when each $f_m^*(x_m)$ is maximized. For $m = 0$ and $m = N$, the optimal condition is trivially achieved when $f_0^* = f_N^* = 1$ with $x_0 = 0$ and $x_N = L$, respectively. Moreover, due to symmetry, the situation with $m = 1$ is equivalent to that with $m = 2$, so it is enough to consider the work of only $m = 1$ of (1), i.e.
Figure 5 shows that at low temperature, $W_1$ of the quantum SZE containing three bosons is negative at the force balance at $x_1 = x_1^0 \approx 0.443L$. However, the positive optimal work is obtained at $x_1 = x_1^{op} \approx 0.490L$, where two curves $F_1(x_1)$ and $(F_2(x_1))^p$ cross. Figure 5(b) shows that for higher temperature, $W_1$ is positive and $x_1^{op}$ comes closer to $x_1^0$. As temperature increases quantum partition functions approach the corresponding classical ones, as does $\sum f_m$, which implies $(F_p(y))^p \rightarrow 0$ as $T \rightarrow \infty$ according to (10). Figure 6 shows for both three bosons and three fermions $x_1^{op}$ approaches $x_1^0$ and finally converges to the classical result, $L/3$, as temperature increases.

So far, we have removed the wall in an isothermal way. As a final remark, let us consider what happens if an adiabatic process is exploited for the wall removal. More precisely, we remove the barrier of the 1-D quantum SZE containing three bosons first adiabatically from $V = \infty$ to $V = V_a$ and then isothermally from $V = V_a$ to $V = 0$. Figure 7 shows that the work extracted is not maximized at $V_a = \infty$, which implies that the quantum SZE done with only isothermal processes is not optimal. However, we emphasize that once the adiabatic process comes into play, the system is no longer in equilibrium. The reason is that as $V$ varies, the energy levels generally move with different rates, i.e. $\frac{\partial E_m}{\partial V} = \frac{\partial E_n}{\partial V}$ $(m \neq n)$, while the corresponding occupation probabilities, $P_m$ and $P_n$, remain intact. As such, temperature is neither kept constant nor even well-defined [12]. It is no surprise that work is extracted from this engine even without invoking information entropy since the conditions of a single reservoir with a single temperature of the SZE have already been broken in the context of Carnot’s principle.

6. Summary

In summary, we have found the optimal conditions of the work done by a quantum SZE with exhibits inevitable irreversibility. The optimal conditions are achieved if the so-called restorability, defined as the probability that
the reversibility of an engine with inevitable irreversibility is achieved when the time-backward process is performed, is maximized. It is equivalent to the condition that the force of time-forward process at the stage, where the irreversibility occurs, is equivalent to that of time-backward. This is important since the force of time-backward always vanishes in classical case due to detailed balance but not in quantum one. At high temperature limit, the force of time-backward thus approaches zero, so that it recovers classical behavior. We confirm our finding by using a quantum SZE containing three bosons or three fermions.

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