Optimal work of quantum Szilard engine

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We have found the optimal condition of the work performed by the quantum Szilard engine (SZE) containing multi-particles. Usually the optimal work of a cyclic engine is achieved when the whole thermodynamic process is reversible. Although the quantum SZE inherently contains an irreversible process, we can still define effectively reversible protocol based upon the force of time-forward and time-backward processes.

Maxwell was the first man that asked a deep physical question on the nature of information using his famous demon [1]. Szilard then recognized the connection between information and entropy, which is demonstrated by his thought experiment called as the Szilard engine (SZE) [2]. It tells us that one can extract work from a cyclic engine with a single heat bath 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, but the Carnot's principle is necessary to modify [3]. The SZE has been realized in various experiments [4–7].

The thermodynamic cycle of the SZE containing N particles in the one-dimensional box of the length L consists of four stages as shown in Fig. 1; (i) to insert a wall at $x = l$ ($0 \leq l \leq L$), (ii) to measure how many particles are in the left side, whose outcome is expressed as m, (iii) to perform isothermal expansion, where the wall stops at $x = x_m^0$ differing in m, and (iv) to remove the wall to complete the cycle. It has been found that the quantum mechanical work done by the SZE is given by [8]

$$W = -k_B T \sum_{m=0}^{N} f_m(l) \ln \left[\frac{f_m(l)}{f_m^\star(x_m)} \right] \quad (1)$$

with $f_m(l) = Z_m(l)/Z(l)$, $f_m^\star(x_m) = Z_m(x_m)/Z(x_m)$ and $Z(y) = \sum_m Z_m(y)$. Here $Z_m(y)$ denotes the partition function of the case that m particles are in the left side of the wall, i.e. $N - m$ particles in the right, when the wall is located at y. Note that l is freely chosen when the wall is inserted, while x_m^0 is determined from the force balance, $F^{\mathrm{L}} + F^{\mathrm{R}} = 0$. The generalized force of the left (right) side of the wall is defined as

$$F^{\mathrm{L(R)}} = \sum_n P_n^{\mathrm{L(R)}} \left[\frac{\partial E_n^{\mathrm{L(R)}}}{\partial x} \right], \quad (2)$$

where $P_n^{\mathrm{L(R)}}$ and $E_n^{\mathrm{L(R)}}$ represent the occupation probability and the eigenenergy of the nth energy level of the left (right) side, respectively.

The work of the *classical* SZE is also expressed as Eq. (1), which is derived by using the dissipative work
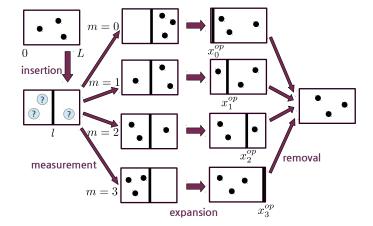

Figure 1. Schematic diagram of the thermodynamic processes of the quantum SZE. (See the text for the details.)

theorem of *classical* non-equilibrium thermodynamics [9]. The reason why the non-equilibrium thermodynamics is taken into account is that it is an irreversible process that the wall separating particles into two parts is removed. This is nothing but free expansion. Even though both quantum and classical SZE have the equivalent mathematical form of the work, Eq. (1), the partition functions differ in classical and quantum mechanics so that the amount of work of the quantum SZE is distinct from that of the classical one [9]. Note that information itself is inherently classical both in the quantum [8] and in the classical SZE [9]. Recently the heat engine exploiting purely quantum information is proposed [10].

Strangely enough in the quantum SZE, however, it has been found that the work of Eq. (1) in the low-temperature limit can be negative as shown in Fig. 2, implying one should do work on the engine instead of extracting work from it [11]. Later it is found that it is not optimal to stop the wall at the force balance originally proposed in Ref. [12]. Instead one can numerically find the optimal condition. In a usual heat engine, the optimal condition of work gain is achieved when the whole thermodynamic process is reversible. As far as the quan-
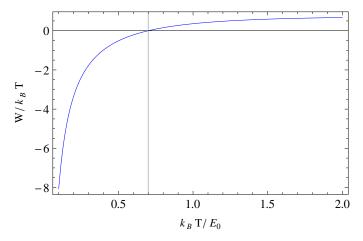
Figure 2. The work of the quantum SZE containing three bosons with $l = L/2$ as a function of temperature when the wall stops at x_m^0 (the force balance point). For low temperature the work becomes negative.

tum SZE is concerned, however, it is unlikely to make it fully reversible since the stage of removing the wall is inherently irreversible as mentioned above. It raises a question on what the physical meaning of the optimal condition of the quantum SZE is.

In this paper we show the optimal work gain of the quantum SZE is achieved if we stop and remove the wall at the location where the force on the wall of the time-forward process is equivalent to the *average* force right after inserting the wall for the *time-backward* process. Note that the time-backward process of removing the wall is simply inserting the wall. For the time-backward process after inserting the wall one cannot automatically return to the original state of the time-forward process, i.e. m particles in the left, since it is an irreversible process to remove the wall in the time-forward process. Thus it is a reasonable way to define the force of the time-backward as the average over all possible cases with different m. Briefly speaking, the optimal condition is then achieved when the time-forward force is equivalent to the time-backward force. In some sense this effectively recovers the reversibility of the inherently irreversible heat engine not because the process itself is reversible but because the forces are reversible. It gives us a new insight on the optimal condition of *irreversible* heat engines.

The work of Eq. (1) is a function of l and $\{x_m\}$ with $m = 0, 1, \cdots, N$, namely $W(l, \{x_m\})$. The optimal (maximum) condition is thus obtained from $\partial W/\partial l = 0$ and $\partial W/\partial x_m = 0$ [13]. From Eq. (1) the latter is shown to be $\partial \ln f_m^\star(x_m)/\partial x_m = 0$, which is also rewritten as

$$\frac{1}{Z_m} \frac{\partial Z_m}{\partial x_m} = \frac{1}{Z} \frac{\partial Z}{\partial x_m} \tag{3}$$

with $Z(y) = \sum_m Z_m(y)$. The partition function Z_m is given as

$$Z_m(y) = \sum_\sigma e^{-\beta \epsilon_m^\sigma(y)} \tag{4}$$

with $\epsilon_m^\sigma = \sum_n (E_n^L m_n^\sigma + E_n^R q_n^\sigma)$, where m_n^σ and q_n^σ represent the number of particles occupying the nth energy level of the left and the right side, respectively, satisfying $m = \sum_n m_n^\sigma$ and $N - m = \sum_n q_n^\sigma$. Here σ denotes the configuration of particles over all the energy levels for a given m.

The left-hand side of Eq. (3) represents the net force on the wall multiplied by the inverse temperature when m particles are in the left side due to

$$\frac{1}{Z_m} \frac{\partial Z_m}{\partial x_m} = -\beta \left\langle \frac{\partial \epsilon_m^\sigma}{\partial x_m} \right\rangle_\sigma \equiv \beta F_m \tag{5}$$

with $\beta = 1/k_B T$. Note that $F_m(x_m^0) = 0$ gives rise to the force balance condition. On the other hand, the right-hand side of Eq. (3) is expressed as

$$\frac{1}{Z} \frac{\partial Z}{\partial x_m} = \frac{1}{Z} \sum_p \frac{\partial Z_p}{\partial x_m} = -\beta \sum_p \frac{Z_p}{Z} \left\langle \frac{\partial \epsilon_p^\sigma}{\partial x_m} \right\rangle_\sigma \equiv \beta \langle F_p \rangle_p. \tag{6}$$

The force $\langle F_p \rangle_p$ of Eq.(6) is obtained from averaging F_p. It is emphasized that every F_p is calculated with the equivalent x_m at which F_m of Eq. (5) is obtained. To understand the physical meaning of this force let us consider the time-forward and back-ward process of removing the wall in detail. Note that the time-backward process of removing the wall is inserting it. For the time-forward the number of particles on the left, m, is determined once the measurement is performed, and then is kept constant before we stop the wall at x_m and remove it. For the time-backward, however, one finds m to vary from 0 to N when the wall is inserted at x_m. $\langle F_p \rangle_p$ is regarded as the legitimate average force at x_m for the time-backward since we inevitably confront such a situation when we perform the reverse thermodynamic process of the quantum SZE.

From Eqs. (5) and (6), the optimal condition Eq. (3) reads

$$F_m(x_m^{\mathrm{op}}) = \langle F_p(x_m^{\mathrm{op}}) \rangle_p. \tag{7}$$

The optimal x_m^{op} is obtained from the condition that the force of the time-forward is equivalent to that of the time-backward. It gives an insight on the optimal condition of the heat engine containing an irreversible process. Usually the optimal work of a heat engine is attained if the whole thermodynamic process is performed in a reversible way. Equation (7) tells us that the *thermodynamically irreversible* quantum SZE becomes optimal if the process is *effectively* reversible, i.e. the forces are reversible. The force is important since the work, which we intend to make optimal, is given by integrating force over coordinate.

The work at the optimal condition is positive. It is recalled that the observation that the work obtained from the force balance, $F_m(x_m^0) = 0$, can become negative in the low temperature initiates this research. Mathematically f_m is equivalent to $f_m^\star$ in their form, namely $f_m(y) = f_m^\star(y)$. Since the optimal work is obtained from
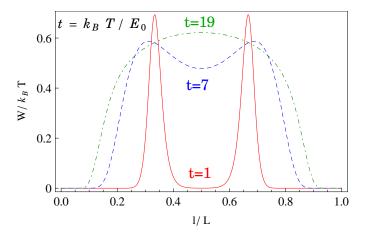
Figure 3. The work W of the SZE containing two spinless fermions as a function of l with various T.

maximizing $f_m^\star$ [See Eq. (1)], i.e. $\partial \ln f_m^\star(x_m)/\partial x_m = 0$, we find $f_m(l) = f_m^\star(l) \leq f_m^\star(x_m^{\mathrm{op}})$ irrespective of l. It immediately implies that the work of Eq. (1) at maximum is positive.

In fact, it is the quantum effect that x_m^0 of the force balance differs from x_m^{op} of the optimal condition. If we consider classical particles satisfying ideal gas law implying pressure is proportional to density, one finds

$$\langle F_p(y) \rangle_p = \sum_{p=0}^{N} P(p) \left(\frac{p}{y} - \frac{N-p}{L-y} \right) = 0 \qquad (8)$$

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

$$P(p) = \left(\frac{y}{L} \right)^p \left(\frac{L-y}{L} \right)^{N-p} \binom{N}{p}. \qquad (9)$$

The optimal condition is thus achieved simply by the force balance since the right-hand side of Eq. (7) always vanishes. Note that x_m^0 of the classical particles are different from that of the quantum ones; They coincide only in the high temperature limit. This will be discussed below in detail.

In some sense it looks weird to have $\langle F_p(x_m^{\mathrm{op}}) \rangle_p \neq 0$ in quantum mechanics. This is simply the net force exerted on a wall when we insert the wall into a box containing particles kept in equilibrium during the process in time-backward process. The non-zero net force cannot be spontaneously developed as far as only quasi-static process of inserting the wall is concerned in classical thermodynamics. We emphasize that it is the quantum effect. Interestingly this seems to be similar to the Casimir effect [14]. If the wall is inserted at $x \neq L/2$, the structures of energy levels of the left and the right sides become different so do the corresponding generalized forces of Eq. (2), namely $\sum_n P_n^{\mathrm{L}}(\partial E_n^{\mathrm{L}}/\partial x)$ and $\sum_n P_n^{\mathrm{R}}(\partial E_n^{\mathrm{R}}/\partial x)$.

So far we have discussed the optimal condition of $\{x_m\}$. The optimal condition of l is rather subtle. Intuitively one expects the symmetric point $l = L/2$ satisfies the
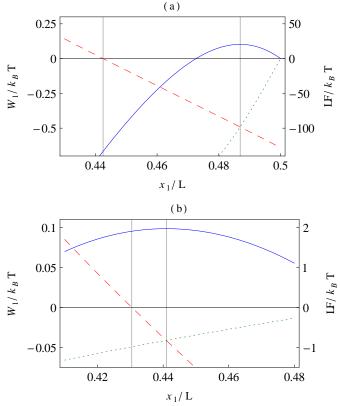
Figure 4. The partial work $W_1(L/2, x_1)$ (the solid curve; see the left hand side of y axis) of the SZE containing three bosons as a function of x_1 for (a) $k_B T/E_0 = 1$ and (b) $k_B T/E_0 = 5$. The dashed and the dotted curves represent $F_1(x_1)$ and $\langle F_p(x_1) \rangle_p$ (see the right hand side of y axis), respectively. The former crosses x axis at x_1^0 denoted by the left vertical line, and intersects the latter at x_1^{op} denoted by the right vertical line.

optimal condition. At least we can 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 $x_m = x_m^{\mathrm{op}}$ since x_m^{op} has nothing to do with l. Then we obtain from $\partial W/\partial l = 0$

$$\langle W_m(l, x_m^{\mathrm{op}}) F_m(l) \rangle_m = \langle W_p(l, x_p^{\mathrm{op}}) \rangle_p \langle F_q(l) \rangle_q \qquad (10)$$

with $W_m(l, y) = -\ln[f_m(l)/f_m^\star(y)]$. Both the left and the right hand sides of Eq. (10) vanishes at $l = L/2$ according to $f_{N-m}(L/2) = f_m(L/2)$, $W_{N-m}(L/2, x_{N-m}^{\mathrm{op}}) = W_m(L/2, x_m^{\mathrm{op}})$ and $F_{N-m}(L/2) = -F_m(L/2)$, so that the work exhibits an extremum at $l = L/2$. However, this is not a unique solution. For example, Figure 3 shows that a single maximum of the work of the SZE containing two spinless fermions splits into two peaks as temperature decreases although the work remains extremum at $l = L/2$. This splitting is associated with the accidental degeneracies of the problem and the exclusion principle of fermions [15]. The optimal co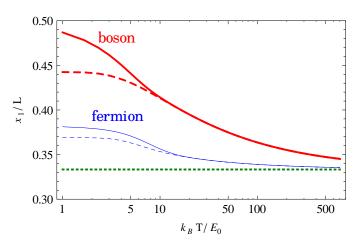ndition of the work of l thus depends on tem-