Quantum Analog of Carnot Engine

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Abstract

In order to build a quantum analog of traditional Carnot engine, a common choice is replacing the two thermodynamic adiabatic processes with two quantum mechanical adiabatic processes. In general, such quantum Carnot engine has six strokes. We analyze the efficiency of such six-stroke quantum Carnot engine in a perturbative way. The analytic analysis matches the numerical result in [5].

1 Introduction

In classical thermodynamics, a Carnot engine consists of two isothermal processes and two thermodynamic adiabatic processes. When trying to establish a quantum mechanical analog of traditional Carnot engine, we identify the counterparts of these thermodynamic processes, and then patch them to build a quantum Carnot engine (abbreviated as QCE) [2, 3].

So how to establish these counterparts? For isothermal process, we identify quantum mechanical isothermal process in a statistical mechanical way by requiring the populations of the substance to satisfy Boltzmann distribution with a fixed temperature [3]. As for adiabatic process, a common choice is replacing thermodynamic adiabatic process \( dQ = \sum_n E_n dP_n = 0 \) with quantum mechanical adiabatic process \( dP_n = 0 \) [1, 3]. We want to emphasize that a quantum mechanical adiabatic process is conceptually different from a
thermodynamic adiabatic process. This fundamental difference is the origin of the differences between traditional Carnot engine and QCE, as we will see in the following.

In classical thermodynamics, if a system is initially at thermal equilibrium, it will still be at thermal equilibrium at the end of a thermodynamic adiabatic process. On the other hand, quantum mechanical adiabatic process doesn’t enjoy such property. Consider a system undergoes a quantum mechanical adiabatic process from state $G$ (at thermal equilibrium with temperature $T_G$) to state $H$. For populations, we have $P_n(G) = P_n(H)$ for all energy levels. Condition for state $H$ being at thermal equilibrium with temperature $T_H$ is

$$E_n(H) - E_m(H) = \frac{T_H}{T_G} (E_n(G) - E_m(G)),$$

(1)

for all $n$ and $m$. Since Eq.(1) is not always satisfied, quantum mechanical adiabatic process doesn’t necessarily bring a thermal equilibrium state to another thermal equilibrium state.

Thermal equilibrium is preserved if Eq.(1) is respected, that is, scale invariance is satisfied. Examples of this kind include a harmonic oscillator with the varied parameter being the harmonic frequency [1, 4], a particle in an infinite square well potential with the varied parameter being the width of the potential well [2].

If Eq.(1) is not satisfied, state $H$ is not at thermal equilibrium. In this case, when the working medium (of state $H$) contacts the thermal reservoir, we get an additional relaxation process (working medium to be thermalized by the reservoir). The cycle thus has six strokes, as shown in Fig. 1. Apparently, traditional Carnot engine and such six-stroke QCE have many differences, including their efficiencies. What we are going to do is studying the efficiency and its optimization of the six-stroke QCE.

2 Efficiency of the quantum Carnot engine and the working medium being considered

Following the discussion of such six-stroke QCE in [5], the efficiency is

$$\eta = 1 - \frac{Q_1}{Q_2} = 1 - \frac{T_1(S_B - S_D) + T_1\Delta S_{C'\to C}^{total}}{T_2(S_B - S_D) - T_2\Delta S_{A'\to A}^{total}},$$

(2)

where $\Delta S^{total}$ is the total entropy increase of the universe.

We can see that $\eta$ differs from Carnot efficiency, due to the existence of the relaxation processes. By the second law of thermodynamics, both $\Delta S_{C'\to C}^{total}$ and $\Delta S_{A'\to A}^{total}$ cannot be neg-
Figure 1: Six-stroke quantum Carnot engine. $A \rightarrow B$ and $C \rightarrow D$ are isothermal processes; $B \rightarrow C'$ and $D \rightarrow A'$ are adiabatic processes; $C' \rightarrow C$ and $A' \rightarrow A$ are relaxation processes; $T_1$ and $T_2$ are the temperatures of the cold reservoir and the hot reservoir, respectively; $\langle E \rangle$ is the mean energy of the system. For simplicity, we assume there is only one system parameter tunable in the cycle operation, called $\lambda$.

ative, and hence $\eta$ is lower than Carnot efficiency. Standard Carnot engine has an universal efficiency, the Carnot efficiency, no matter what are its working substance and the thermal reservoirs. On the contrary, efficiency of six-stroke QCE depends on the detail of the working substance.

In this paper, we consider six-stroke QCE whose degree of nonequilibrium is small. That is, the scenario is the six-stroke QCE perturbed around ordinary four-stroke Carnot engine. The spectrum of the working medium being considered is

$$E_n = \lambda f(n) + \alpha g(n),$$

where $f(n)$ has no degeneracy. Here $\lambda$ is the system parameter tuned in the cycle operations; $\alpha$ is a small constant, and the term $\alpha g(n)$ aims to break the scale invariance and thus lead
to the two relaxation processes. The six-stroke QCE reduces to ordinary four-stroke Carnot engine when $\alpha = 0$, and $\lambda$ is denoted as $\lambda^0$ in this case. Our goal is maximizing the efficiency (in a perturbative way) with $\lambda_C$ and $\lambda_A$, while $T_1$, $T_2$, $\lambda_B$ and $\lambda_D$ are fixed. We consider $\delta \lambda_C$ and $\delta \lambda_A$ to be of order $\alpha$. That is,

$$\lambda = \lambda^0 + \alpha \lambda^1.$$  

By construction, $\lambda_B^1 = \lambda_D^1 = 0$, $\lambda_C = \lambda_C^0 + \alpha \lambda_C^1$, $\lambda_A = \lambda_A^0 + \alpha \lambda_A^1$.

Our work is inspired by \cite{5}. The paper considers some general discussion, and then the numerical result of a special case. Different from \cite{5}, here we analyze systems whose spectrums are described by Eq.(3). Since we take an analytic approach, $\alpha$ needs to be small enough such that perturbation can work appropriately.

### 3 Calculation of heat exchange

Let’s calculate $Q_1$ and $Q_2$, with energy levels specified by Eq.(3). In this work, perturbation is kept to $O(\alpha^2)$. Symbolically, the zeroth order of population and the zeroth order of partition function are denoted as $P_n^0$ and $Z^n_0$, respectively.

For $\alpha = 0$, there is no relaxation process, and hence $P_n^0(B) = P_n^0(C)$ and $P_n^0(D) = P_n^0(A)$. Furthermore, by Eq.(1), we obtain

$$\beta \lambda_B = \beta_1 \lambda_C^0, \hspace{1em} \beta \lambda_D = \beta_2 \lambda_A^0,$$

where $\beta \equiv \frac{1}{k_B T}$. Define $\langle O \rangle$ as the average of $O_n$ weighted by $P_n^0$:

$$\langle O \rangle \equiv \sum_n P_n^0 O_n.$$  

Then define inner product as

$$\langle O_1 | O_2 \rangle \equiv \langle O_1 O_2 \rangle - \langle O_1 \rangle \langle O_2 \rangle = \langle (O_1 - \overline{O_1}) (O_2 - \overline{O_2}) \rangle,$$

where $\overline{O} \equiv \langle O \rangle$.

Calculate $Q_1$ via $Q_1 = \langle E_C' \rangle - \langle E_D \rangle + k_B T_1 (\ln Z_C - \ln Z_D)$ and $Q_2$ via $Q_2 = \langle E_B \rangle - \langle E_A' \rangle + k_B T_2 (\ln Z_B - \ln Z_A)$ to $O(\alpha^2)$. We get
\[ Q_1 \approx \left[ \frac{\beta_2}{\beta_1} \lambda_B \langle f \rangle_B - \lambda_D \langle f \rangle_D + \frac{1}{\beta_1} (\ln Z_B^0 - \ln Z_D^0) \right] \\
+ \alpha \left[ - \frac{\beta_2^2}{\beta_1} \lambda_B \langle f \mid g \rangle_B + \beta_1 \lambda_D \langle f \mid g \rangle_D \right] \\
+ \alpha^2 \left[ - \beta_2 \langle g \mid g \rangle_B + \frac{1}{2} \beta_1 (\langle g \mid g \rangle_B + \langle g \mid g \rangle_D) \right] \\
+ \frac{\alpha^2}{2} \left[ - \beta_2 \lambda_B \left( \langle g \rangle_B \langle f \mid g \rangle_B - \frac{1}{2} \langle f \mid g^2 \rangle_B \right) + \beta_1^2 \lambda_D \left( \langle g \rangle_D \langle f \mid g \rangle_D - \frac{1}{2} \langle f \mid g^2 \rangle_D \right) \right] \\
+ \alpha^2 \left[ - (\beta_2 - \beta_1) \lambda_C^1 \langle f \mid g \rangle_B + \frac{1}{2} \beta_1 (\lambda_C^1)^2 \langle f \mid f \rangle_B \right], \tag{8} \]

\[ Q_2 \approx \left[ \lambda_B \langle f \rangle_B - \frac{\beta_1}{\beta_2} \lambda_D \langle f \rangle_D + \frac{1}{\beta_2} (\ln Z_B^0 - \ln Z_D^0) \right] \\
+ \alpha \left[ - \beta_2 \lambda_B \langle f \mid g \rangle_B + \frac{\beta_1}{\beta_2} \lambda_D \langle f \mid g \rangle_D \right] \\
+ \alpha^2 \left[ - \frac{1}{2} \beta_2 \langle g \mid g \rangle_B + \langle g \mid g \rangle_D + \beta_1 \langle g \mid g \rangle_D \right] \\
+ \frac{\alpha^2}{2} \left[ - \beta_2 \lambda_B \left( \langle g \rangle_B \langle f \mid g \rangle_B - \frac{1}{2} \langle f \mid g^2 \rangle_B \right) + \frac{\beta_1^2}{\beta_2} \lambda_D \left( \langle g \rangle_D \langle f \mid g \rangle_D - \frac{1}{2} \langle f \mid g^2 \rangle_D \right) \right] \\
+ \alpha^2 \left[ - (\beta_2 - \beta_1) \lambda_A^1 \langle f \mid g \rangle_D - \frac{1}{2} \beta_1 (\lambda_A^1)^2 \langle f \mid f \rangle_D \right]. \tag{9} \]

We can see that the variations of \( \lambda_C \) and \( \lambda_A \) don’t alter \( Q_1 \) and \( Q_2 \) until \( O(\alpha^2) \), which implies that \( \eta = 1 - T_1/T_2 \) up to \( O(\alpha) \). The feature will be discussed in the following.

4 Analysis of efficiency and its optimization

Now let’s analyze \( \eta \) order by order.

4.1 Zeroth order

By Eq.(8) and Eq.(9), the zeroth order term of the efficiency is given by

\[ \eta = 1 - \frac{T_1}{T_2}, \tag{10} \]
as expected.

### 4.2 First order

Keep the efficiency to \( O(\alpha) \) and we have

\[
\eta = 1 - \frac{T_1}{T_2}.
\] (11)

The first order term also gives Carnot efficiency. Why?

Consider that state \( G \), which is almost at thermal equilibrium with temperature \( T \), undergoes a thermalization process by contacting with a reservoir of temperature \( T \), and then reaches state \( H \). We have \( P_n(G) = P_n(H) + \delta P_n \), where \( \delta P_n \) is small. Calculate \( \Delta S_{G \rightarrow H}^{\text{total}} \) to the second order of \( \delta P_n \) and we obtain

\[
\Delta S_{G \rightarrow H}^{\text{total}} \approx \frac{1}{2} k_B \sum_n \frac{(\delta P_n)^2}{P_n(H)}.
\] (12)

This is exactly what the second law of thermodynamics tells us. Entropy has maximum at thermal equilibrium, which is state \( H \) in our case, and hence its first order expansion due to small departure vanishes. Furthermore, for a spontaneous process, the total entropy cannot decrease, and hence \( \Delta S_{G \rightarrow H}^{\text{total}} \) is positive definite.

Due to the second law of thermodynamics, both \( \Delta S_{C \rightarrow C}^{\text{total}} \) and \( \Delta S_{A' \rightarrow A}^{\text{total}} \) have vanishing first order terms. Therefore, there is no efficiency correction up to \( O(\alpha) \) (by Eq.(2)).

### 4.3 Second order

Now let’s turn to the second order term. Minimize \( Q_1 \) with \( \lambda_C^1 \) and maximize \( Q_2 \) with \( \lambda_A^1 \), and we get the maximum of the efficiency

\[
\eta = \left(1 - \frac{T_1}{T_2}\right) + \alpha^2 \left[-\frac{1}{2} \frac{\beta_2}{\beta_1} (\beta_1 - \beta_2)^2 \right] \left[\frac{\langle g \mid g \rangle - \langle f \mid g \rangle^2}{\langle f \mid f \rangle} \right]_B + \left[\frac{\langle g \mid g \rangle - \langle f \mid g \rangle^2}{\langle f \mid f \rangle} \right]_D.
\] (13)

This is the final result of the efficiency of the six-stroke QCE under optimization with respect to \( \lambda_C^1 \) and \( \lambda_A^1 \).

If the physics makes sense, we should be able to prove mathematically that \( \eta \) is always not bigger than \( 1 - T_1/T_2 \). Here is the proof. First, \( \beta_2 Q_2^0 \) is positive and hence \( \beta_2 \lambda_B \langle f \rangle_B -
\[ \beta_1 \lambda_D \langle f \rangle_D + (\ln Z_B^0 - \ln Z_D^0) \] is positive. Second, by Cauchy-Schwarz inequality, \[ \langle g \mid g \rangle \langle f \mid f \rangle - \langle f \mid g \rangle^2 \geq 0. \] Therefore, the efficiency is always not bigger than \( 1 - T_1/T_2 \).

In the following, we have four observations for the second order correction of the efficiency. These tendencies can be seen in the numerical example of [5] (Figure 2 in [5]).

**Observation 1:** In our setting, \( \lambda_D \) should be bigger than \( \lambda_0 \) in order to guarantee \( Q_1 > 0 \), which can be seen from Fig. 1. By Eq.(5), we have

\[ \beta_2 \lambda_B < \beta_1 \lambda_D. \]  \hspace{1cm} (14)

It is unphysical considering \((\lambda_B, \lambda_D)\) with \( \beta_2 \lambda_B > \beta_1 \lambda_D \).

**Observation 2:** For \( \beta_2 \lambda_B \approx \beta_1 \lambda_D \), the isothermal processes are short, and hence the nonequilibrium effect of the relaxation processes becomes significant. For a fixed \( \beta_1 \lambda_D \), the efficiency decreases sharply as \( \beta_2 \lambda_B \) approaching its maximum \( (\beta_1 \lambda_D) \); for a fixed \( \beta_2 \lambda_B \), the efficiency decreases sharply as \( \beta_1 \lambda_D \) approaching its minimum \( (\beta_2 \lambda_B) \).

**Observation 3:** Consider the limiting case of

\[ \beta \lambda \gg 1, \] \hspace{1cm} (15)

which corresponds to low temperature or high energy scale. Consider only the contributions of the two lowest energy levels (two-level system) as an approximation, and then we get

\[ \langle g \mid g \rangle - \frac{\langle f \mid g \rangle^2}{\langle f \mid f \rangle} \approx 0. \] \hspace{1cm} (16)

Take Eq.(16) into Eq.(13), and we can see that efficiency correction goes to zero for \( \beta \lambda \gg 1 \). This tendency can be understood by the fact that a two-level system can always be regarded as being at thermal equilibrium.

**Observation 4:** Consider the limiting case of

\[ \beta \lambda \ll 1, \] \hspace{1cm} (17)

which corresponds to high temperature or low energy scale. In this case, \( P_n \) approaches a constant as \( \beta \lambda \) goes to zero. So efficiency correction also approaches a constant as \( \beta \lambda \) goes to zero.
5 Conclusions

We analyze some properties of the six-stroke QCE. The features of the six-stroke QCE come from the replacement of thermodynamic adiabatic process with quantum mechanical adiabatic process. It is a non-trivial step, and the meaning of such replacement is still an open question. We hope that we can have conceptual understanding of such QCE and quantum thermodynamics in the future.

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