

QUANTUM-MECHANICAL ANALOG OF THE CARNOT CYCLE: GENERAL FORMULA FOR EFFICIENCY AND MAXIMUM-POWER OUTPUT

Sumiyoshi Abe

Department of Physical Engineering, Mie University, Mie 514-8507, Japan

ABSTRACT

The quantum-mechanical Carnot cycle is an analog of the thermodynamic one and is constructed without heat baths. The cycle is realized by controlling quantum states of particles as well as a confining potential. Here, recent developments about such a cycle are reported. The general formula for the efficiency is presented for an arbitrary potential. A finite-time process is also discussed, and the value of the efficiency under the maximum power condition is derived in the case of a one-dimensional infinite square-well potential.

INTRODUCTION

Small systems are of interest from various viewpoint in contemporary science. In particular, the problems of constructing microscopic machines/engines and understanding their operating mechanisms are relevant to biology (e.g., biomolecular motors), information theory (e.g., Maxwell's demon), nanoscience and so on.

The subject of the present article is concerned with a reversible engine made of a single quantum-mechanical particle confined in an variable potential. This system does not contain heat baths, and the volume change (i.e., expansion and compression) is realized by external control of the potential. Accordingly, quantum coherence remains intact. In Ref. [1], it has been shown, by considering a cycle of a system consisting of a particle in an infinite square-well potential with the movable walls, that it is in fact possible to construct a reversible cycle and to extract work from it. The cycle constructed there is analogous to Carnot's, and is therefore referred to as *quantum-mechanical Carnot cycle*. However, because of the absence of hot and cold heat baths, it should not be confused with cycles of genuine quantum heat engines discussed in the literature (see, for example, Refs. [2-7]).

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The cycle is described in Fig. 1. We discuss a case, which is much more general than that in Ref. [1].

Initially, the system is in a state, $|u_1(V_A)\rangle$, at A. After the volume expansion, the system reaches B in a higher state, say $|u_2(V_B)\rangle$. During the expansion process $A \rightarrow B$, the system is in a superposed state, $a_1(V)|u_1(V)\rangle + a_2(V)|u_2(V)\rangle$

$(|a_1(V)|^2 + |a_2(V)|^2 = 1)$, but the average energy (i.e., an analog of the internal energy) $E_H \equiv \langle H \rangle_H = \sum_{n=1,2} E_n(V) |a_n(V)|^2$ is kept unchanged. Here, $H = H(V)$

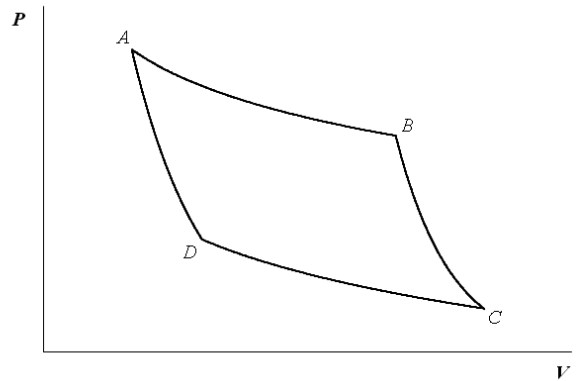


Figure 1. The cycle depicted in the plane of volume V and pressure P .

is the system Hamiltonian for the stationary Schrödinger equation, $H(V)|u_n(V)\rangle = E_n(V)|u_n(V)\rangle$, which is valid under the adiabaticity condition, that is, slow change of V . The time scale of change of V is much larger than that of the dynamical one, $\sim \hbar / E$, with E being a typical value of the energy. Note that $E_H = E_1(V_A) = E_2(V_B)$ and $a_1(V_B) = a_2(V_A) = 0$. Similar is the process $C \rightarrow D$, in which the state changes from $|u_2(V_C)\rangle$ to $|u_1(V_D)\rangle$, and in-between it is a superposed one,

$b_1(V)|u_1(V)\rangle + b_2(V)|u_2(V)\rangle$ ($|b_1(V)|^2 + |b_2(V)|^2 = 1$), but the average energy $E_L \equiv \langle H \rangle_L = \sum_{n=1,2} E_n(V) |b_n(V)|^2$ is kept unchanged. We have $E_L = E_2(V_C) = E_1(V_D)$ and $b_1(V_C) = b_2(V_D) = 0$. These two processes are analogs of the isothermal processes in the thermodynamic Carnot cycle. On the other hand, $B \rightarrow C$ and $D \rightarrow A$ are analogs of the adiabatic processes. During $B \rightarrow C$ ($D \rightarrow A$), the state remains as $|u_2(V)\rangle$ ($|u_1(V)\rangle$). These analogies have been clarified in Ref. [8] from the viewpoint of a formal similarity between quantum mechanics and thermodynamics. An explicit example using a one-dimensional infinite square-well potential with movable walls shows [1] that it is in fact possible to construct a cycle of this kind.

Work is defined by $d'W = \langle \partial H(V) / \partial V \rangle dV \equiv -P dV$, where P is pressure. The work during each process is given as follows: $W_{AB} = \int_{V_A}^{V_B} dV \sum_{n=1,2} [\partial E_n(V) / \partial V] |a_n(V)|^2$, $W_{BC} = \int_{V_B}^{V_C} dV \partial E_2(V) / \partial V$, $\int_{V_C}^{V_D} dV \sum_{n=1,2} [\partial E_n(V) / \partial V] |b_n(V)|^2$ and $W_{DA} = \int_{V_D}^{V_A} dV \partial E_1(V) / \partial V$. It can be shown [9] that $W_{BC} = -W_{DA}$ holds, in general. Therefore, the work extracted after a single cycle is $W = W_{AB} + W_{BC} + W_{CD} + W_{DA} = W_{AB} + W_{CD}$. The efficiency of the cycle is then given by $\eta = W / W_{AB}$. In Ref. [9], the following general formula for the efficiency has been presented:

$$\eta = 1 - \frac{\int_{V_D}^{V_C} dV \Delta E(V) \frac{\partial}{\partial V} \left[\frac{E_L - \bar{E}(V)}{\Delta E(V)} \right]}{\int_{V_A}^{V_B} dV \Delta E(V) \frac{\partial}{\partial V} \left[\frac{E_H - \bar{E}(V)}{\Delta E(V)} \right]} \quad (1)$$

where

$$\bar{E}(V) = \frac{1}{2} [E_1(V) + E_2(V)], \quad (2)$$

$$\Delta E(V) = E_2(V) - E_1(V). \quad (3)$$

Eq. (1) shows how the efficiency depends on the structure of the energy spectrum. Since a potential is the analog of a working material in thermodynamics, this formula exhibits how the quantum-mechanical Carnot cycle is nonuniversal. This is due to the fact that, in pure-state quantum mechanics, the von Neumann entropy identically vanishes and, therefore, there does not exist an analog of the second law of thermodynamics.

Closing this section, we would like to mention an intriguing point regarding the efficiency in Eq. (1) for a certain class of spectra. Suppose the energy eigenvalues to have the form

$$E_n(V) = \frac{\varepsilon_n}{V^\alpha} \quad (n = 1, 2, 3, \dots) \quad (4)$$

where α and ε_n 's are independent of V , $\alpha > 0$ and $\varepsilon_1 < \varepsilon_2 < \varepsilon_3 < \dots$. The spectra of this form are referred to here as *homogeneous type*. In this case, Eq. (1) is calculated to have the following simple form:

$$\eta = 1 - \frac{E_L}{E_H}. \quad (5)$$

A homogeneous-type spectrum will be discussed in the next section.

FINITE-TIME PROCESSES AND MAXIMUM POWER OUTPUT

So far, we have seen the nonuniversal nature of the quantum-mechanical Carnot cycle. Here, we wish to examine this point from a different aspect. Specifically, we consider finite-time processes and the condition for the maximum power output [10]. For this purpose, we employ a simple system of a particle confined in a one-dimensional infinite square-well potential as in Ref. [1]. The energy eigenvalues are given by $E_n(L) = n^2 \pi^2 \hbar^2 / (2mL^2)$ ($n = 1, 2, 3, \dots$), where L is the width of the potential well and slowly changes in time. (Since the system is one-dimensional, L corresponds to the volume V in the preceding section.) We note that this spectrum is of the homogeneous type. Taking the ground ($n = 1$) and first excited ($n = 2$) states and applying Eq. (5), we obtain

$$\eta = 1 - 4 \left(\frac{L_A}{L_C} \right)^2, \quad (6)$$

where L_A and L_C are the values of the potential width at A and C , respectively.

Now, let $v(t)$ be the speed of the change of the width. The total amount of movement of L during a single cycle is given by

$$L_{\text{total}} = 2(L_C - L_A) = \int_0^\tau dt v(t) \equiv \bar{v} \tau, \quad (7)$$

where τ is the cycle time and \bar{v} is the average speed. Eq. (7) allows one to express the cycle time as follows:

$$\tau = \frac{2}{\bar{v}} (L_C - L_A). \quad (8)$$

On the other hand, the work extracted after a single cycle is $W = (\pi^2 \hbar^2 / m) (1/L_A^2 - 4/L_C^2) \ln 2$. The condition

$$r \equiv \frac{L_C}{L_A} > 2 \quad (9)$$

has to be fulfilled in order for the work extracted to be positive. The power output is then expressed as follows [10]:

$$\Pi \equiv \frac{W}{\tau} = \frac{\pi^2 \hbar^2 \bar{v} \ln 2}{2mL_A^3} \cdot \frac{r^2 - 4}{r^3 - r^2}. \quad (10)$$

Our interest is in maximization of Π . This problem turns out to be given by the solution of the equation, $r^3 - 12r + 8 = 0$. This cubic equation has three real solutions, but $r = 4 \cos(2\pi/9)$ is the one and only solution consistent with the condition in Eq. (9). Then, the corresponding value of the efficiency is

$$\eta^* = 1 - \frac{1}{4 \cos^2(2\pi/9)} = 0.573977952\dots \quad (11)$$

This result is *universal* in the sense that it does not contain any of the parameters characterizing the system under consideration.

CONCLUSION

We have reported recent developments made about the quantum-mechanical Carnot cycle. We have discussed the general formula derived for the efficiency for an arbitrary potential confining a particle. Also, we have mentioned the result on the efficiency under the maximum power condition by employing a one-dimensional infinite square-well potential.

As stressed in the very beginning of this article, the systems' quantum coherence remains intact, since no heat baths are present. This fact leads to the following question: Can the principle of superposition plays some role here? The answer to this question seems to be affirmative. It is in fact shown in Ref. [11] that the efficiency can be enhanced by superposition of relevant states. It is also of extreme interest to examine roles and effects of quantum entanglement in systems consisting of more than one particle.

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