WORK OUTPUT AND EFFICIENCY OF A REVERSIBLE QUANTUM OTTO CYCLE

by

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An idealized reversible Otto cycle working with a single quantum mechanical particle contained in a potential well is investigated based on the Schrödinger equation in this paper. The model of a reversible quantum Otto cycle, which consists of two reversible adiabatic and two constant-well widen branches, is established. As an example, we calculate a particularly simple case in which only two of the eigenstates of the potential well contribute to the wave-function in the well. The relationship between the optimal dimensionless work output W^* vs. the efficiency η for the two-eigenstate system is derived. The efficiency of this quantum cycle is shown to equal that of a classical reversible Otto cycle because quantum dynamics is reversible.

Key words: *quantum Otto cycle, wave-function, optimal work output, efficiency*

Introduction

A heat engine is an important energy conversion device. A classical heat engine converts heat energy into mechanical work by means of a gas that expands and pushes a piston in a cylinder. For a classical thermodynamic heat engine the energy required is generally from a high-temperature heat reservoir. Its work output and efficiency may be obtained by the first law of thermodynamics and the classical ideal gas equation of state. However, a quantum heat engine [1-20] obeys the laws of quantum mechanics. The influence of the quantum characteristics of the working fluid on the performance of the cycle must be considered.

The quantum heat engine attracts much attention due to its special features. Present technology now allows for the probing and/or realization of quantum mechanical systems of microscopic and even macroscopic sizes (like those of superconductors, Bose-Einstein condensates, *etc*.) which can also be restricted to a relatively small number of energy states. It is interesting that the quantum cycles analyzed can be similar to various aspects of classical thermodynamic cycles such as Carnot [18, 20], Stirling [5, 7, 21], Otto [22-24], Brayton [16, 17,

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25], and Ericsson [19, 26] cycles. To investigate the characteristics of a quantum cycle certain methods such as the quantum degeneracy theory [21-23], the semi-group approach [1, 2], the Schrödinger equation [17-18], and the quantum master equation [4-5] have be adopted.

The Otto cycle is one of the typical thermodynamic cycles. Much work has been performed for the performance analysis and optimization of either the classical [27-29] or quantum [22-24] Otto engine. In this paper we construct an idealized reversible Otto heat engine that consists of a single quantum mechanical particle contained in a potential well. We allow the walls of the confining potential to play the role of the piston by moving in and out. The system we discuss here is a single quantum particle in a potential well. The working fluid of a real Otto engine consists of an infinite number of copies of such particles, each in its own potential well. Explicitly, the only principles we need are those of the Schrödinger equation, the Born probability interpretation of the wave functions.

The work out was found for a reversible quantum Carnot heat engine by solving the Schrödinger equation in reference [18], but the maximum work out was not derived. In this paper, the work out and the efficiency are derived for a reversible quantum Otto heat engine that consists of two reversible adiabatic and two constant-well widen branches by solving the Schrödinger equation. The maximum work output and the relationship between the optimal dimensionless work output W^* *vs.* the efficiency for the two-eigenstate system is obtained.

Quantum dynamics of the engine system

Let us consider a particle of mass m confined to a one-dimensional infinite square well of width L. The time-independent Schrödinger equation for this system is [30]:

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + \frac{2mE}{\hbar^2}\psi = 0 \tag{1}$$

where m and E are the mass and the energy of a particle, respectively, the $\psi(x)$ is wave-function required to satisfy the boundary conditions $\psi(0) = 0$ and $\psi(L) = 0$. Planck's constant $\eta = 6.63\cdot10^{-34}$ [Js] and $\hbar = \eta/2\pi = 1.05\cdot10^{-34}$ [Js] in the system solving eq. (1) gives:

$$\psi(x) = \sum_{n=1}^{\infty} a_n\phi_n(x) \tag{2}$$

with

$$\phi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi}{L}x\right) \tag{3}$$

where $\phi_n(x)$ are the normalized eigenstates of this system and the coefficients a_n satisfy the normalization condition:

$$\sum_{n=1}^{\infty}|a_n|^2 = \sum_{n=1}^{\infty}p_n = 1 \tag{4}$$

where $p_n = |a_n|^2$ $(n = 1, 2, \cdots\cdots, \infty)$ are the corresponding occupation probabilities of the system. The eigenvalues E_n corresponding to the eigenstates $\phi_n(x)$ is:

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} \tag{5}$$

The expectation value of the Hamiltonian of the system $E = \langle\psi|H|\psi\rangle$ is:

$$E = \sum_{n=1}^{\infty} |a_n|^2 E_n = \sum_{n=1}^{\infty} p_n E_n \tag{6}$$

where H is the Hamiltonian of the system. Let us now suppose that one of the infinite walls of the potential well, say the wall at $x = L$, can move like the piston in a one-dimensional cylinder for a classical thermodynamic system [18]. If this wall is allowed to move an infinitesimal amount dL, then the wave-function $\psi(x)$, the eigenstates $\phi_n(x)$, and energy levels all vary infinitesimally as functions of L. As a consequence, the expectation value of the Hamiltonian E also changes infinitesimally.

Quantum Otto cycle

It is well know that the Otto cycle is made of two isochoric branches connected by two adiabatic branches. We consider the following cyclic process as shown in fig. 1. We start from state 1 with a wave-function in a well of width L_1.

In process 1-2, keeping the widen L_1 constant, the system gains some energy by some kind of contact with a heat bath. The system jumps up from the lower energy level E_1 to the upper energy level E_2. Only energy is pumped into the system in this stage to yield a change in the occupation probabilities. In process 2-3, we allow the system to expand adiabatically from $L = L_1$ until $L = L_2$. In an adiabatic process, the size of the potential well changes as the wall moves. The system is isolated from the heat bath and undergoes a quantum adiabatic expansion to reduce the energy from E_2 to a smaller value E_3. An amount of work is thus performed by the system, but no heat is transferred. In process 3-4, keeping the widen L_2 constant, the system releases some energy to the environment by some kind of contact with another heat bath. The system evolves from the upper energy level E_3 to the lower energy level E_4 by the energy transition. Only energy is released into the environment in this stage to yield a change in the occupation probabilities. In process 4-1, we compress the system adiabatically from $L = L_2$ until we return to the starting point $L = L_1$. In this stage, the system is removed from the heat bath and undergoes a quantum adiabatic contraction to increase the energy level from E_4 back to the larger value E_1. An amount of work is performed on the system.

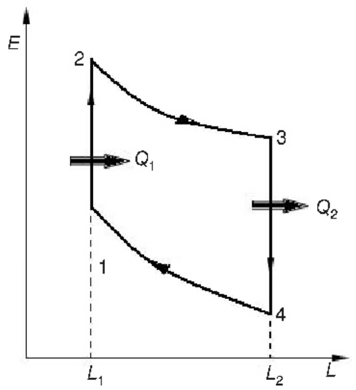

Figure 1. A quantum Otto cycle consisting of four steps, two isothermal processes and two adiabatic processes. The cycle is shown as a closed loop in the *E-L* plane

The cycle 1-2-3-4 is a reversible quantum Otto cycle. Note that we need not and have not assigned temperature to a single quantum mechanical particle. The temperatures are properties of the energy which are assumed to be in the Gibbs state.

Output work and efficiency

From eq. (6) these expectation values of the Hamiltonian at state 1, state 2, state 3, and state 4 may be written as:

$$E_1 = \sum_{n=1}^{\infty} p_{1n} \frac{n^2\pi^2\hbar^2}{2mL_1^2} = \frac{\pi^2\hbar^2}{2mL_1^2} \sum_{n=1}^{\infty} n^2 p_{1n} \tag{7}$$

$$E_2 = \sum_{n=1}^{\infty} p_{2n} \frac{n^2\pi^2\hbar^2}{2mL_1^2} = \frac{\pi^2\hbar^2}{2mL_1^2}\sum_{n=1}^{\infty} n^2 p_{2n} \tag{8}$$

$$E_3 = \sum_{n=1}^{\infty} p_{3n} \frac{n^2\pi^2\hbar^2}{2mL_2^2} = \frac{\pi^2\hbar^2}{2mL_2^2}\sum_{n=1}^{\infty} n^2 p_{3n} \tag{9}$$

$$E_4 = \sum_{n=1}^{\infty} p_{4n} \frac{n^2\pi^2\hbar^2}{2mL_2^2} = \frac{\pi^2\hbar^2}{2mL_2^2}\sum_{n=1}^{\infty} n^2 p_{4n} \tag{10}$$

where E_1, E_2, E_3, and E_4 are the expectation values of the Hamiltonian at state 1, state 2, state 3, and state 4, respectively, and p_{1n}, p_{2n}, p_{3n}, and p_{4n}, are the transition probabilities of the system from state n to state 1, state 2, state 3, and state 4, respectively. In process 1-2, the energy supplied by the environment is:

$$Q_1 = E_2 - E_1 = \frac{\pi^2\hbar^2}{2mL_1^2}\sum_{n=1}^{\infty} n^2 (p_{2n} - p_{1n}) \tag{11}$$

In process 3-4, the energy released to the environment is:

$$Q_2 = E_3 - E_4 = \frac{\pi^2\hbar^2}{2mL_2^2}\sum_{n=1}^{\infty} n^2 (p_{3n} - p_{4n}) \tag{12}$$

Based on the first law of thermodynamics, combining eqs. (11) and (12) gives the net work output of our quantum heat engine:

$$W = Q_1 - Q_2 = \frac{\pi^2\hbar^2}{2mL_1^2}\sum_{n=1}^{\infty} n^2 \left(\frac{p_{2n} - p_{1n}}{L_1^2} - \frac{p_{3n} - p_{4n}}{L_2^2}\right) \tag{13}$$

The efficiency of the engine cycle $\eta = W/Q_1$ is:

$$\eta = 1 - \frac{L_1^2 \sum_{n=1}^{\infty} n^2 (p_{3n} - p_{4n})}{L_2^2 \sum_{n=1}^{\infty} n^2 (p_{2n} - p_{1n})} \tag{14}$$

Equations (13) and (14) give the work output and the efficiency. It is the main result of this paper.

Two-state quantum heat engine

In this paragraph we consider a particularly simple case for convenience in which only two of the eigenstates of the potential well contribute to the wave-function described blow in the well. From eq. (2) the wave-function of the two-eigenstate system can be written as:

$$\psi(x) = a_1\sqrt{\frac{2}{L}}\sin\left(\frac{\pi}{L}x\right) + a_2\sqrt{\frac{2}{L}}\sin\left(\frac{2\pi}{L}x\right) \tag{15}$$

with

$$|a_1|^2 + |a_2|^2 = p_1 + p_2 = 1 \tag{16}$$

In the quantum adiabatic expansion process 2-3 and the quantum adiabatic compression process 4-1, since the expansion/compression rate is sufficiently slow the system remains in equilibrium at all times. The absolute values of the occupation probabilities must remain constant according to the quantum adiabatic theorem [17-18, 30]. The cycle of the heat engines then puts a constraint on the probabilities:

$$p_{3n} = p_{2n}, \quad p_{4n} = p_{1n} \tag{17}$$

From eqs. (13), (14), (16), and (17) the work output and the efficiency for a two-state quantum heat engine may be written as:

$$W = \frac{3\pi^2\hbar^2}{2m}\left(\frac{1}{L_1^2} - \frac{1}{L_2^2}\right)(p_{41} - p_{21}) \tag{18}$$

$$\eta = 1 - \frac{L_1^2}{L_2^2} \tag{19}$$

If the two-eigenstates system is allowed to couple to the heat baths in process 1-2 and process 3-4, the thermal equilibrium probabilities with the thermal equilibrium Gibbs distributions may be written as [17]:

$$p_{21} = [1 + \exp(\pi^2\hbar^2/2mL_1^2)/kT_2]^{-1} \tag{20}$$

$$p_{41} = [1 + \exp(\pi^2\hbar^2/2mL_2^2)/kT_4]^{-1} \tag{21}$$

where p_{21}, and p_{41} are transition probabilities of the system from state 1 to state 2, and state 4, respectively. T_2 and T_4 are the temperature of the gas, which consists of an infinite number of copies of such particles each in its own potential well, at state 2 and at state 4, respectively. These probabilities are definitely non-zero. Thus, eq. (18) can be rewritten as:

$$W = \frac{3\pi^2\hbar^2(x^2 - 1)}{2mL_2^2}\left\{\left[1 + \exp\left(\frac{\pi^2\hbar^2}{2kmT_4L_2^2}\right)\right]^{-1} - \left[1 + \exp\left(\frac{\pi^2\hbar^2x^2}{2kmT_2L_2^2}\right)\right]^{-1}\right\} \tag{22}$$

with $x = L_2/L_1$. Substituting eq. (19) into eq. (22) yields:

$$W = \frac{3\pi^2\hbar^2\eta}{2mL_2^2(1-\eta)}\left\{\left[1 + \exp\left(\frac{\pi^2\hbar^2}{2kmT_4L_2^2}\right)\right]^{-1} - \left[1 + \exp\left(\frac{\pi^2\hbar^2}{2kmT_4L_2^2}\frac{1}{1-\eta}\right)\right]^{-1}\right\} \tag{23}$$

where k is the Boltzmann's constant.

The eq. (23) gives the fundamental relationship between the work output W and efficiency η of a two-state quantum heat engine for the given parameters L_2, T_2, and T_4.

It is clearly seen from eq. (23) that work output W of the engine is function of L_2 for given parameters η, T_2, and T_4. Taking the derivatives of W with respect to L_2 and setting it equal zero, one can find that when $L_2 = L_{20}$ satisfies the equation:

$$\begin{aligned}&\left[1 + \left(1 - \frac{\pi^2\hbar^2}{2kmT_4L_{20}^2}\right)\exp\left(\frac{\pi^2\hbar^2}{2kmT_4L_{20}^2}\right)\right]\left[1 + \exp\left(\frac{\pi^2\hbar^2}{2kmT_2L_{20}^2}\frac{1}{1-\eta}\right)\right]^2 = \\ &\left[1 + \left(1 - \frac{\pi^2\hbar^2}{2kmT_4L_{20}^2}\frac{1}{1-\eta}\right)\exp\left(\frac{\pi^2\hbar^2}{2kmT_2L_{20}^2}\right)\right]\left[1 + \exp\left(\frac{\pi^2\hbar^2}{2kmT_4L_{20}^2}\right)\right]^2\end{aligned} \tag{24}$$

The work output approaches optimal value:

$$W_0 = \frac{3\pi^2\hbar^2\eta}{2mL_{20}^2(1-\eta)}\left\{\left[1+\exp\left(\frac{\pi^2\hbar^2}{2kmT_4L_{20}^2}\right)\right]^{-1}-\left[1+\exp\left(\frac{\pi^2\hbar^2}{2kmT_2L_{20}^2}\frac{1}{1-\eta}\right)\right]^{-1}\right\} \tag{25}$$

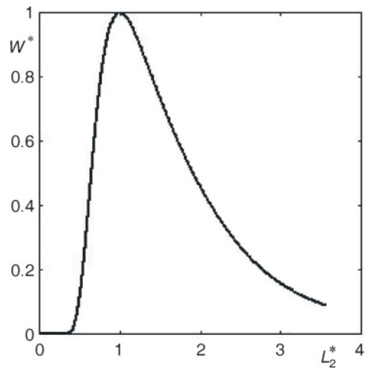

Figure 2. The Dimensionless work output W^* *vs.* the dimensionless potential well with L_2^*

The W^* *vs.* L_2^* characteristic with $p^2\hbar^2/2kmT_4 = 0.1$ and $T_4/(1-\eta)T_2 = 12$ is shown in fig. 2, where $W^* = W/W_0$ is the dimensionless work output and $L_2^* = L_2/L_{20}$ is the dimensionless potential well width. From fig. 2 one can see clearly that there exist the maximum work output $W = W_0$ corresponding to $L_2 = L_{20}$. Obviously, for different given parameters the maximum work output will be different.

The W_1^* *vs.* η characteristic with $p^2\hbar^2/2kmT_4L_2^2 = 1.278$ and $T_4/T_2 = 0.75$ is shown in fig. 3, where $W_1^* = 2mL_2^2W/3\pi^2\hbar^2$. It may be seen from fig. 3 that the work output increases with the increase in the efficiency η. The reason is that our quantum heat engine is a reversible one.

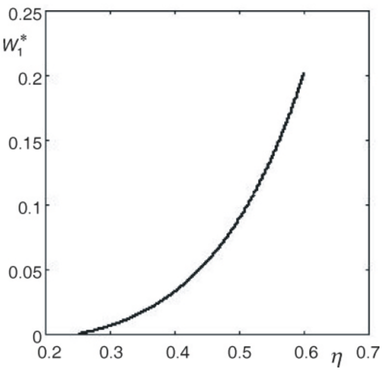

Figure 3. The dimensionless work output W_1^* *vs.* the efficiency η

Discussion

The force F exerted on the wall of the well is given by:

$$F = -\frac{dF}{dL} \tag{26}$$

Combining eqs. (5), (6), and (26) yields:

$$F = \sum_{n=1}^{\infty} p_n \frac{n^2\pi^2\hbar^2}{mL^3} \tag{27}$$

From eqs. (17) and (27), the forces in processes 2-3 and 4-1 can be written, respectively, as:

$$F_{23} = \sum_{n=1}^{\infty} p_{2n} \frac{n^2\pi^2\hbar^2}{mL^3} \tag{28}$$

$$F_{41} = \sum_{n=1}^{\infty} p_{1n} \frac{n^2\pi^2\hbar^2}{mL^3} \tag{29}$$

Based on eqs. (28) and (29) , we can now obtain the output work, too:

$$W = \int_{L_1}^{L_2} F_{23}dL + \int_{L_2}^{L_1} F_{41}dL = \frac{\pi^2\hbar^2}{2m}\sum_{n=1}^{\infty} n^2\left(\frac{p_{2n}-p_{1n}}{L_1^2}-\frac{p_{3n}-p_{4n}}{L_2^2}\right) \tag{30}$$

As our expectation, eq. (30) is in agreement on eq. (13).

Because our quantum Otto engine consisting of a single quantum mechanical particle is reversible, the influence of the potential well width L would be important. It is seen from eqs.

(13) and (14) that both the work output and the W efficiency η of the reversible quantum Otto cycle increase with the increase in L_2/L_1.

It is well known that the efficiency of the reversible Otto engine whose working fluid is composed classical idea gases is:

$$\eta = 1 - \frac{V_1^{\gamma-1}}{V_2^{\gamma-1}} \tag{31}$$

where γ is the ratio of specific heats, and V_1 and V_2 are, respectively, the minimum volume and the maximum volume of the gas in the cylinder.

For a particle confined to a one-dimensional infinite square well as mentioned above, its number of freedom i equates 1. We have:

$$\gamma = \frac{i+2}{i} = 3 \tag{32}$$

Substituting $\gamma = 3$ into eq. (31) yields $\eta = 1 - (V_1^2/V_2^2)$. It shows that the efficiency of a reversible two-eigenstate quantum Otto cycle is the same as that of a classical reversible Otto cycle.

Conclusion

In this paper, we proposed the model of a reversible quantum Otto cycle, which consists of two reversible adiabatic and two constant-well widen branches. The work output and the efficiency of the cycle are investigated by solving the Schrödinger equation. The two-eigenstate system is calculated as an example. The relationship between the optimal dimensionless work output W^* *vs.* the efficiency η is derived for a two-eigenstate heat engine. The efficiency of this quantum cycle is shown to equal that of the reversible Otto engine whose working fluid is composed classical idea gases because quantum dynamics is reversible.

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