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2000 J. Phys. A: Math. Gen. 33 4427

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Quantum mechanical Carnot engine

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Received 15 November 1999, in final form 6 April 2000

Abstract. A cyclic thermodynamic heat engine runs most efficiently if it is reversible. Carnot constructed such a reversible heat engine by combining adiabatic and isothermal processes for a system containing an ideal gas. Here, we present an example of a cyclic engine based on a single quantum mechanical particle confined to a potential well. The efficiency of this engine is shown to equal the Carnot efficiency because quantum dynamics is reversible. The quantum heat engine has a cycle consisting of adiabatic and isothermal quantum processes that are close analogues of the corresponding classical processes.

1. Introduction

A thermodynamic heat engine converts heat energy into mechanical work by means of a gas that expands and pushes a piston in a cylinder. A heat engine obtains its energy from a high-temperature heat reservoir. Some of the energy taken from this reservoir is converted to useful mechanical work. However, because a heat engine is not perfectly efficient some of the energy taken from the heat reservoir is *not* converted to mechanical energy, but rather is transferred to a low-temperature reservoir.

The efficiency of a heat engine is defined as follows [1]. If an amount of heat energy Q_H is taken from the high-temperature reservoir and an amount W of mechanical work is obtained, then the efficiency η of the heat engine is defined to be

$$\eta = \frac{W}{Q_H}. \quad (1)$$

The amount of heat deposited in the low-temperature reservoir is Q_C , which by conservation of energy is given by

$$Q_C = Q_H - W. \quad (2)$$

It is easy to show that a heat engine running between a given pair of high-temperature and low-temperature reservoirs achieves maximum efficiency if it is *reversible*. Of course, in practice it is impossible to construct a heat engine that is perfectly reversible. However, Carnot, in the early 19th century, proposed an ideal mathematical model of a heat engine that is not only reversible but also cyclic [2]. The Carnot engine consists of a cylinder of ideal gas that is alternately placed in thermal contact with the high-temperature and low-temperature heat

reservoirs whose temperatures are T_H and T_C , respectively. Carnot showed that the efficiency η of such a reversible heat engine is

$$\eta = 1 - \frac{T_C}{T_H}. \quad (3)$$

The Carnot cycle consists of four processes, each of which is reversible. First, the gas in the cylinder undergoes an isothermal expansion at temperature T_H while it is in contact with the high-temperature reservoir. Second, the gas continues to expand adiabatically in thermal isolation until its temperature drops to T_C . Third, the gas is compressed isothermally in contact with the low-temperature reservoir. Fourth, the gas is compressed adiabatically until its temperature rises to T_H .

In this paper we construct an idealized reversible heat engine that consists of a single quantum mechanical particle contained in a potential well. Rather than having an ideal gas in a cylinder, we allow the walls of the confining potential to play the role of the piston by moving in and out. We show that there exist the quantum equivalents of isothermal and adiabatic reversible thermodynamic processes. However, in place of the temperature variable in classical thermodynamics, we use the energy as given by the pure-state expectation value of the Hamiltonian. Not surprisingly, since this engine is a reversible engine, its efficiency is identical to the classical result in equation (3) with T replaced by the expectation value of the Hamiltonian.

In our formulation, we do not use the concept of temperature. In a classical thermodynamic system, such as an ideal gas in a cylinder, the temperature is determined by the average velocity of the large number of gas molecules. The system we discuss here is a single quantum particle in a potential well. To interpret such a system we think of having an infinite number of copies of such particles, each in its own potential well. We replace the role of temperature, which is an average, by the expectation value of the Hamiltonian, that is, the ensemble average of the energies of the quantum particle. Thus, the quantum analogue of keeping our quantum ensemble in contact with a heat bath as the walls of the potential move is to maintain, by some unspecified physical means, the constancy of the expectation value of the Hamiltonian.

This paper is organized as follows. In section 2 we describe various kinds of quantum processes that may be undergone by a particle confined to a potential well and we explain how to perform reversible quantum expansions and compressions. Next, in section 3 we combine these processes to formulate a reversible cyclic quantum heat engine. We show that this quantum heat engine is the precise analogue of a classical heat engine running on a *monatomic* ideal gas. Finally, in section 4 we make some general remarks concerning quantum heat engines and discuss some differences between classical and quantum heat engines.

2. Adiabatic, free, and isothermal quantum processes

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

$$-\frac{\hbar^2}{2m}\psi''(x) - E\psi(x) = 0 \quad (4)$$

where $\psi(x)$ is required to satisfy the boundary conditions $\psi(0) = 0$ and $\psi(L) = 0$. A general solution to this equation can be expressed as a linear combination of eigenfunctions $\phi_n(x)$:

$$\psi(x) = \sum_{n=1}^{\infty} a_n \phi_n(x) \quad (5)$$

where the coefficients a_n satisfy the normalization condition

$$\sum_{n=1}^{\infty} |a_n|^2 = 1. \quad (6)$$

The normalized eigenstates $\phi_n(x)$ of this system are

$$\phi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right) \quad (n = 1, 2, 3, \dots) \quad (7)$$

and the corresponding eigenvalues E_n are

$$E_n = \frac{\pi^2 \hbar^2 n^2}{2mL^2} \quad (n = 1, 2, 3, \dots). \quad (8)$$

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. If this wall is allowed to move an infinitesimal amount dL , then the wavefunction $\psi(x)$, eigenstates $\phi_n(x)$, and energy levels all vary infinitesimally as functions of L . As a consequence, the expectation value of the Hamiltonian $E(L) = \langle \psi | H | \psi \rangle$ also changes infinitesimally. It is natural to define the force on the wall of the potential well as the negative derivative of the energy. Hence, the force F exerted on the wall of the well is given by $F = -\frac{dE(L)}{dL}$.

Based on this force, we can now define several kinds of processes which are the quantum analogues of classical thermodynamic processes.

2.1. Adiabatic process

Classically, an adiabatic process is one in which the system is thermally isolated. Thus, for a gas in a cylinder, heat cannot flow into or out of the gas. In this process the piston moves but the system remains in equilibrium at all times. As the piston moves, the gas in the cylinder does work. Thus, some of the internal energy of the gas is converted into mechanical energy. Let us suppose that the gas in the cylinder is a monatomic one-dimensional ideal gas. The equation of state of this gas is $PV = NkT$ and the internal energy U of the gas is $U = \frac{1}{2}NkT$. The mechanical work dW done by an infinitesimal expansion dV of the gas is given by $dW = P dV$. By definition, in an adiabatic expansion $dU + dW = 0$. Solving this differential equation gives the standard result that characterizes an adiabatic process:

$$PV^3 = C \quad (9)$$

where C is a constant.

We assume that the initial quantum state $\psi(x)$ of a particle in a square well of width L is a linear combination of eigenstates as in equation (5). In an adiabatic process, the size of the potential well changes as the wall moves. Since the system remains in equilibrium at all times, the absolute values of the expansion coefficients $|a_n|$ must remain constant [3]. That is, we do not expect any transitions between states to occur during an adiabatic process. However, it is clear from equations (7) and (8) that, as L changes, the eigenstates $\phi_n(x)$ and corresponding energy eigenvalues E_n all vary smoothly as functions of L .

Each energy eigenvalue decreases as the piston moves out (as L increases), so the expectation value of the Hamiltonian

$$E(L) = \sum_{n=1}^{\infty} |a_n|^2 E_n \quad (10)$$

where E_n is given in (8), also decreases as a function of L . The energy that is lost equals the mechanical work done by the force F , which is given by

$$F(L) = \sum_{n=1}^{\infty} |a_n|^2 \frac{\pi^2 \hbar^2 n^2}{mL^3}. \quad (11)$$

Note that, during an adiabatic process, the phase of the wavefunction of the particle changes, even though the particle remains fixed in a given eigenstate. This, however, does not affect the results in this paper, because we are only interested in expectation values which are independent of phases.

2.2. Free expansion

Classically, a free expansion is one in which the piston suddenly moves outward. The gas in the cylinder instantly departs from equilibrium and expands to fill the new volume. During this process the system remains isolated from any heat source, so heat energy cannot flow into or out of the gas in the cylinder. Since the piston is not pushed outward by the gas, the system does no work. Thus, the internal energy in the gas remains constant during this process. The temperature of an ideal gas is proportional to the internal energy of the gas, and thus the equation that characterizes a free expansion process is

$$T = C \quad (12)$$

where C is a constant. Also, after the expansion of the gas when equilibrium is restored, the final pressure has decreased relative to the initial pressure in such a way that $P_{\text{final}} V_{\text{final}} = P_{\text{initial}} V_{\text{initial}}$.

Quantum mechanically, in a free expansion the initial state $\psi(x)$ of the system of volume L becomes a final state for which the expectation value of the Hamiltonian is the same as its initial expectation value. This is the quantum analogue of the requirement that the internal energy remain the same during a free expansion because the system does no mechanical work.

At the new value of L , say αL , where $\alpha > 1$, we have a new set of eigenfunctions $\chi_n(x)$ of the form

$$\chi_n(x) = \sqrt{\frac{2}{\alpha L}} \sin\left(\frac{n\pi}{\alpha L}x\right) \quad (n = 1, 2, 3, \dots). \quad (13)$$

After the expansion, each of the initial eigenstates ϕ_n becomes a linear combination of the eigenstates $\chi_m(x)$ associated with the well of width αL :

$$\phi_n = \sum_{m=1}^{\infty} b_{m,n} \chi_m(x) \quad (14)$$

where $b_{m,n}$ is the overlap integral

$$\begin{aligned} b_{m,n} &= \int_0^L dx \phi_n(x) \chi_m(x) \\ &= \frac{2n\alpha^{3/2}(-1)^n}{\pi(m^2 - \alpha^2 n^2)} \sin\left(\frac{m\pi}{\alpha}\right). \end{aligned} \quad (15)$$

Using this formula we can verify that the expectation values of the Hamiltonian in the initial state and in the final state are indeed the same. Suppose that the initial state is in the n th eigenstate. Then, we require

$$\sum_{m=1}^{\infty} b_{m,n}^2 E_m(\alpha L) = E_n(L)$$

to hold for an arbitrary integer n and arbitrary $\alpha > 1$. Using equation (15) for $b_{m,n}$, this can be written as

$$\sum_{m=1}^{\infty} \frac{4\alpha m^2}{\pi^2(m^2 - \alpha^2 n^2)^2} \sin^2\left(\frac{m\pi}{\alpha}\right) = 1. \tag{16}$$

To verify this identity, we note that it can be rewritten more simply as

$$\left[\frac{\alpha}{\pi^2} \left(n \frac{\partial}{\partial n} + 2 \right) \sum_{m=1}^{\infty} \frac{1}{m^2 - \alpha^2 n^2} \left(1 - \cos \frac{2\pi m}{\alpha} \right) \right] \Big|_{n=\text{positive integer}} = 1.$$

Then, to establish this equation we use the general formula

$$\sum_{m=1}^{\infty} \frac{\cos(mx)}{m^2 - u^2} = \frac{1}{2u^2} - \frac{\pi \cos\{(2k+1)\pi - x\}u}{2u \sin(\pi u)}$$

where k is the largest integer such that $2\pi k \leq x$ [4]. Next, we put $x = 2\pi/\alpha$ and $u = \alpha n$ and take $k = 0$ because we have assumed that $\alpha > 1$. It is now easy to show that equation (16) is satisfied.

Note that in the textbook by Schiff [5] it is stated that, when a quantum system undergoes a sudden expansion, the associated energy generally changes. The point that is not stated therein, however, is that the *expectation value* of the Hamiltonian is conserved in such a process, as we have illustrated above.

2.3. Isothermal process

Classically, an isothermal process is one in which, as the piston moves, the system remains in equilibrium at all times. During this process the system is in contact with a heat source so that the temperature T of the gas in the cylinder remains fixed. As the piston moves, the system does work. However, since the temperature of the gas remains constant, the internal energy of the gas also remains constant. Thus, if the equation of state of the gas is $PV = NkT$, then the equation that characterizes an isothermal process is

$$PV = C \tag{17}$$

where C is a constant.

Quantum mechanically, we characterize an isothermal expansion as follows. We assume that the initial state $\psi(x)$ of the system of volume L is a linear combination of eigenstates as in equation (5). In an isothermal process, the size of the potential well changes as the wall moves. However, the expectation value of the Hamiltonian remains constant as the size of the well changes. This expectation value is an ensemble average taken over the multiple copies of the system. Technically speaking, we regard this ensemble as a mixed state; we are not concerned with the phases of the states making up the ensemble. (In principle, constancy of the expectation value of the Hamiltonian may be achieved by pumping energy into the system, possibly by using lasers.) Thus, the expansion coefficients a_n must change in such a way as to keep

$$E(L) = \sum_{n=1}^{\infty} |a_n|^2 E_n \tag{18}$$

fixed as L increases.

The instantaneous force on the piston as a function of L is given by equation (11). However, unlike the adiabatic case, the coefficients $|a_n|^2$ in (11) are now no longer constants, but rather vary as functions of L subject to the constraint that

$$\sum_{n=1}^{\infty} |a_n|^2 = 1. \tag{19}$$

3. Quantum Carnot cycle

Using the quantum adiabatic process and the quantum isothermal process described in section 2 we can now construct a cyclic heat engine. Note that we cannot use a quantum free expansion because this process is not reversible. We consider first a particularly simple case in which only *two* of the eigenstates of the potential well contribute to the wavefunction in the well. Then, we consider the general case in which any number of states participate.

3.1. Two-state quantum heat engine

We consider the following cyclic process. We start with a ground-state wavefunction in a well of width L_1 . At this point the force on the wall is

$$F = \frac{\pi^2 \hbar^2}{mL_1^3}$$

and the expectation value of the Hamiltonian is

$$E_H = \frac{\pi^2 \hbar^2}{2mL_1^2} \quad (20)$$

where the subscript H is in analogy with the T_H in equation (3).

Step 1. We allow the piston to expand isothermally. As we do so, we excite the second energy level of the system, keeping the expectation value of the Hamiltonian constant. Thus, during this isothermal expansion, the state of the system is a linear combination of the lowest two energy eigenstates:

$$\psi(x) = a_1(L) \sqrt{\frac{2}{L}} \sin\left(\frac{\pi}{L}x\right) + a_2(L) \sqrt{\frac{2}{L}} \sin\left(\frac{2\pi}{L}x\right) \quad (21)$$

where, from equation (19), we have $|a_1|^2 + |a_2|^2 = 1$. The expectation value of the Hamiltonian in this state as a function of L is

$$\frac{\pi^2 \hbar^2}{2mL^2} (4 - 3|a_1|^2)$$

where we have used the condition $|a_1|^2 + |a_2|^2 = 1$ to eliminate $|a_2|^2$. Setting the expectation value of the Hamiltonian equal to E_H gives

$$L^2 = L_1^2 (4 - 3|a_1|^2).$$

Thus, the maximum possible value of L in this isothermal expansion is $L_2 = 2L_1$, and this is achieved when $a_1 = 0$. Note that at $L = L_2$ the system is purely in the second energy eigenstate. Along this isothermal expansion the force as a function of L is

$$F_1(L) = |a_1|^2 \frac{\pi^2 \hbar^2}{mL^3} + (1 - |a_1|^2) \frac{4\pi^2 \hbar^2}{mL^3} = \frac{\pi^2 \hbar^2}{mL_1^2 L}. \quad (22)$$

Observe that the product $LF_1(L)$ is a constant. This is the exact quantum analogue of the classical equation of state in equation (17). In general, for a one-dimensional quantum system undergoing an isothermal process, we have

$$LF(L) = C \quad (23)$$

where C is a constant.

Step 2. Next, we allow the system to expand adiabatically from $L = L_2$ until $L = L_3$. During this expansion the system remains in the second state and the expectation value of the Hamiltonian is

$$E_C = \frac{2\pi^2\hbar^2}{mL^2}. \quad (24)$$

The force as a function of L can be taken from equation (11):

$$F_2(L) = \frac{4\pi^2\hbar^2}{mL^3}. \quad (25)$$

The product $L^3 F_2(L)$ is a constant. This is the quantum analogue of the classical equation of state in equation (9). In general, for a one-dimensional quantum system undergoing an adiabatic process, we have

$$L^3 F(L) = C \quad (26)$$

where C is a constant.

Step 3. Third, we compress the system isothermally from $L = L_3$ until $L = L_4$. During this compression we extract energy so that the expectation value of the Hamiltonian remains constant. At the beginning of the compression the system is in its second excited state. We choose to compress the system until it is back in the ground state. At this point $L_4 = \frac{1}{2}L_3$. During this compression the expectation value of the Hamiltonian is kept constant at the value

$$\frac{2\pi^2\hbar^2}{mL_3^2}.$$

The applied force as a function of L is

$$F_3(L) = \frac{4\pi^2\hbar^2}{mL_3^2 L}. \quad (27)$$

Step 4. Finally, we continue to compress the system adiabatically from $L = L_4$ until we return to the starting point $L = L_1$. During this compression the system remains in the ground state and the expectation value of the Hamiltonian is

$$\frac{\pi^2\hbar^2}{2mL^2}.$$

The force applied to the wall of the potential well is given by

$$F_4(L) = \frac{\pi^2\hbar^2}{mL^3}. \quad (28)$$

The four-step cyclic quantum process that we have just described is illustrated in figure 1. The Carnot cycle is drawn in the (F, L) plane, which is the one-dimensional version of the (P, V) plane. The area of the closed loop represents the mechanical work W done in a single cycle of the quantum heat engine. To calculate W we evaluate the following integrals:

$$\begin{aligned} W &= \int_{L_1}^{2L_1} dL F_1(L) + \int_{2L_1}^{L_3} dL F_2(L) + \int_{L_3}^{L_3/2} dL F_3(L) + \int_{L_3/2}^{L_1} dL F_4(L) \\ &= \frac{\pi^2\hbar^2}{m} \left(\frac{1}{L_1^2} - \frac{4}{L_3^2} \right) \ln 2. \end{aligned} \quad (29)$$

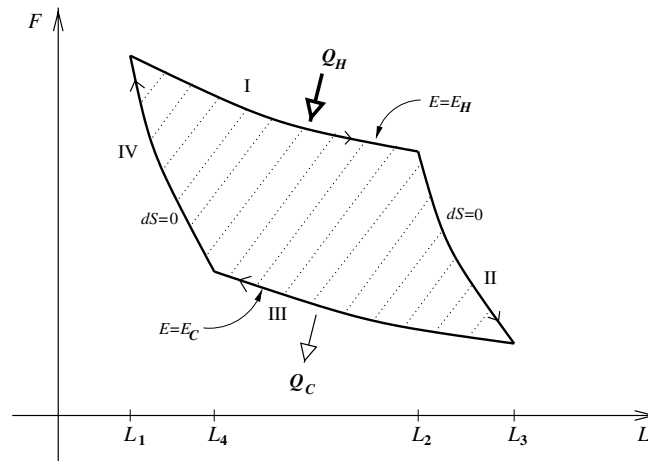


Figure 1. A quantum Carnot cycle consisting of four steps, two isothermal processes and two adiabatic processes. The cycle is shown as a closed loop in the (F, L) plane. The area enclosed in the loop equals the mechanical work done by the engine.

To determine the efficiency of this two-state heat engine we need to calculate the energy absorbed by the potential well during the isothermal expansion. This quantity of energy Q_H is given by

$$\begin{aligned} Q_H &= \int_{L_1}^{2L_1} dL F_1(L) \\ &= \frac{\pi^2 \hbar^2}{L_1^2 m} \ln 2. \end{aligned} \quad (30)$$

Therefore, the efficiency η of our two-state quantum heat engine, as given in the general formula (1), is

$$\eta = 1 - 4 \left(\frac{L_1}{L_3} \right)^2. \quad (31)$$

Using equations (20) and (24), we can rewrite this formula as

$$\eta = 1 - \left(\frac{E_C}{E_H} \right). \quad (32)$$

The energy in this formula plays the role of temperature in equation (3), and thus (32) is the analogue of the classical thermodynamical result of Carnot.

3.2. Multiple-state quantum heat engine

It is straightforward to generalize the two-state quantum Carnot engine to n states. The only change that occurs is that the maximum length of the isothermal expansion increases. Specifically, we find that for n states, if the initial width of the well is L_1 , then the maximum value of L_2 is bounded above by nL_1 .

We note that the entropy S of the quantum system can be defined as

$$S = - \sum_{i=1}^{\infty} |a_i|^2 \ln |a_i|^2 \quad (33)$$

when we drop the constraint to limit the allowable number of states. In this case, the entropy increases during an isothermal expansion, while S decreases for an isothermal compression. On the other hand, for an adiabatic process, the entropy remains fixed because the absolute values $|a_i|$ of the expansion coefficients do not change.

4. Discussion

We have shown that the efficiency of a quantum Carnot cycle is the same as that of a classical Carnot cycle, with the identification of the expectation value of the Hamiltonian as the temperature of the system. However, there is a distinct advantage of a quantum Carnot cycle over a classical Carnot cycle. The heat processes of a classical Carnot cycle must be reversible and therefore the ideal gas in the cylinder must be in equilibrium at all times. If the piston moves with finite speed then the gas is immediately out of equilibrium and the process is no longer reversible. Therefore, it takes an infinitely long time for a classical Carnot engine to complete one cycle.

By contrast, for a quantum Carnot engine, any given cycle lasting a finite time $t > 0$ has a calculable probability of being reversible. For a quantum cycle that lasts an infinite amount of time, during the adiabatic part of the cycle, a particle in a given energy eigenstate remains in that eigenstate. This is true because of the quantum adiabatic theorem [3, 5]. If the adiabatic portion of the cycle lasts a long but finite amount of time, then there is a small but nonzero probability amplitude that the particle may end up in a different energy eigenstate. Thus, there is a large probability that the Carnot cycle is reversible.

To understand the calculation that must be performed, consider step 2 (the adiabatic quantum expansion) of a two-state Carnot engine as described in section 3. For this process, there is a finite probability that there will be no transitions between states during this process. (The specific calculation of this probability is described in [5] and is not of particular interest here.) This probability becomes smaller as the speed of the engine increases, but for a finite-speed quantum Carnot engine, we can make the speed sufficiently slow that this probability becomes negligibly different from unity. Thus, quantum mechanics makes a maximally efficient heat engine an actual physical possibility. Furthermore, because a quantum Carnot engine is reversible, if it follows the cycle in figure 1 in reverse, it functions as a quantum refrigerator. While a classical refrigerator is inherently inefficient, an efficient quantum refrigerator might actually be feasible.

Finally, we must address the question of whether a quantum Carnot cycle is truly cyclic. In the calculations we have done concerning energy, work, force, and efficiency, only the absolute values $|a_n|$ of the expansion coefficients in equation (5) appear. In the quantum Carnot cycle pictured in figure 1 the values of $|a_n|$ are indeed cyclic. However, over the course of a cycle the relative phases of these coefficients can change; each coefficient may accrue a geometric phase contribution. We do not know whether the relative phases have physically observable consequences with regard to the functioning of a quantum heat engine.

Acknowledgments

CMB thanks the Theoretical Physics Group at Imperial College, London, for its hospitality. DCB thanks the Royal Society for financial support. DCB and BKM thank the Physics Department at Washington University for its hospitality. This work was supported in part by the US Department of Energy.

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