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On Cyclic Quantum Heat Engines

Sixth Semester Project Report

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1 Introduction

Description of quantum thermodynamic cycles is a subject filled with deep implications, and allows us investigate the relation between, and the limits to validity of quantum mechanics and thermodynamics. The major portion of this project was dedicated to studying the literature surrounding quantum heat engine cycles, and comparing their properties to their classical counterparts.

In this chapter, we start by looking at the foundational issues in thermodynamics and see that, how for the resolution of these issues, we require information to be physical. The following section summarises some results in information theory that are of interest in the description of quantum heat engines, before moving on to describe Maxwell's demon, the Szilard engine, and Landauer's principle.

1.1 Entropy and information

If we consider an event *A* with possible outcomes $\{a_i\}$ which have an associated probability of occurrence $P(a_i)$, then the *information* obtained by learning that $A = a_j$ in a random trial, is defined $h[P(a_j)] = -K \log P(a_j)$, where the positive constant *K* is to be determined or selected later. It is more useful to associate an amount of information with the event and all its possible outcomes

$$H(A) = -K \sum_{i} P(a_i) \log P(a_i), \qquad (1.1)$$

which is defined by averaging the information associated with each outcome over the set of all outcomes. With $K = k_B$, we recognize (1.1) as the entropy from statistical mechanics.

If we have two events *A* and *B*, with associated outcomes $\{a_i\}$ and $\{b_j\}$ respectively, then for the joint probability distribution $P(a_i, b_j)$ we have

$$H(A,B) = -K \sum_{i,j} P(a_i, b_j) \log P(a_i, b_j),$$
(1.2)

which is the information associated with the events *A* and *B*. Moreover, it can be shown [1] that H(A), H(B), and H(A, B) are constrained by the inequality

$$H(A) + H(B) \ge H(A, B), \tag{1.3}$$

which in particular, ensures that the mutual information defined by

$$H(A:B) = H(A) + H(B) - H(A,B),$$
(1.4)

remains non-negative. The mutual information is a measure of the correlation between events *A* and *B*. In particular, we note that

$$H(A:B) = -K \sum_{i,j} P(a_i, b_j) \log\left(\frac{P(a_i, b_j)}{P(a_i)P(b_j)}\right),$$
(1.5)

vanishes when $P(a_i, b_j) = P(a_i)P(b_j)$, that is when the events are independent. Only if learning the values of *B* changes the probabilities of *A* will the mutual information be non-zero.

1.1.1 Maximum entropy method of assigning probabilities

For real events, the probability distribution $P(a_i)$ must often be determined with limited knowledge of the system, and any bias in selecting the probabilities must be minimized. In order to do this, we select the most uniform distribution that is consistent with what knowledge of the event we do have. In particular, if we know nothing about the event, we should set all probabilities equal. One way to determine the most uniform probability distribution is to maximize the entropy of the event subject to constraints imposed by our knowledge.

For an illustration of this maximum entropy principle, we consider a physical system that can exist in a number of distinct configurations $\{n\}$, with energies $\{E_n\}$. If we are to find probabilities P_n that the system be found in the *n*th configuration, and we are given that the average energy is *U*, we use the *Lagrange multipliers method* to maximise the entropy *H*, subject to constraints $\sum_n P_n = 1$ and $\sum_n P_n E_n = U$.

Lagrange multipliers λ and β are introduced, and quantity

$$\hat{H} = H + \lambda \left(1 - \sum_{n} P_n \right) + \beta \left(U - \sum_{n} P_n E_n \right),$$
(1.6)

where $H = -\sum_{n} P_n \log P_n$, is varied. Varying the probabilities and setting the variation of \hat{H} to zero gives

$$d\hat{H} = \sum_{n} (-\log P_n - 1 - \lambda - \beta E_n) dP_n = 0,$$
(1.7)

the solution of which is $P_n = e^{-(1+\lambda)}e^{-\beta E_n}$. The normalisation condition $\sum_n P_n = 1$, gives $e^{1+\lambda} = \sum_n e^{-\beta E_n}$ and consequently

$$P_n = \frac{e^{-\beta E_n}}{Z(\beta)}, \quad Z(\beta) = \sum_n e^{-\beta E_n}.$$
(1.8)

Moreover, if we put $K = k_B$, identify the information of the probability distribution as the entropy of the system $S = -k_B \sum_n P_n \log P_n$, and recall the thermodynamic relation

$$\frac{\mathrm{d}U}{\mathrm{d}T} = T\frac{\mathrm{d}S}{\mathrm{d}T},\tag{1.9}$$

it can be shown that $\beta = (k_B T)^{-1}$. We defer the proof to the next paragraph and identify $Z(\beta)$ as the *partition function* of the system and the probabilities in (1.8) as the Boltzmann distribution.

In order to show that $\beta = 1/k_B T$, we substitute the probabilities (1.8) into the expression of entropy

$$\frac{S}{k_B} = -\sum_n \frac{e^{-\beta E_n}}{Z(\beta)} [-\beta E_n - \ln Z(\beta)]$$
$$= U\beta + \ln Z, \qquad (1.10)$$

and take its temperature derivative

$$\frac{1}{k_B}\frac{\mathrm{d}S}{\mathrm{d}T} = \beta \frac{\mathrm{d}U}{\mathrm{d}T} + U \frac{\mathrm{d}\beta}{\mathrm{d}T} + \frac{\mathrm{d}\ln Z(\beta)}{\mathrm{d}T}.$$
(1.11)

Next, we note that

$$\frac{d \ln Z(\beta)}{dT} = \frac{1}{Z(\beta)} \frac{dZ(\beta)}{dT}$$

$$= \frac{1}{Z(\beta)} \frac{d}{dT} \sum_{n} e^{-\beta E_{n}}$$

$$= -\frac{d\beta}{dT} \sum_{n} \frac{e^{-\beta E_{n}}}{Z(\beta)} E_{n}$$

$$= -\frac{d\beta}{dT} U,$$
(1.12)

use the thermodynamic relation (1.9) to get

$$\frac{1}{k_B}\frac{\mathrm{d}S}{\mathrm{d}T} = \beta \frac{\mathrm{d}U}{\mathrm{d}T} = \frac{1}{k_B T} \frac{\mathrm{d}U}{\mathrm{d}T},\tag{1.13}$$

and conclude that $\beta = 1/k_B T$.

We see that applying principles of information theory has led us to a fundamental result in thermodynamics. Another example of a connection between information and thermodynamics is *Maxwell's demon*—a thought experiment that calls into question the validity of the second law.

1.2 Maxwell's demon

The setup for this thought experiment involves a box filled with gas at uniform temperature that is divided into two parts L and R. There is a trapdoor between the two parts that is controlled by an *intelligent being*, who can observe the gas molecules near the trapdoor. When the being sees a faster than average molecule approaching the trapdoor from L to R, it allows the molecule to go to R; and when it sees a slower than average molecule approaching the trapdoor from R to L, the being lets it through.



As this process goes on for a sufficiently long time, the average speed of molecules in *L* becomes less

than the average speed of molecules in R. According to the kinetic theory of gases, the average speed of molecules is proportional to the temperature. Hence, due to the being's actions the temperature in L decreases while the temperature in R increases, against the temperature gradient.

This apparent violation of the second law of thermodynamics can be resolved if there is a physical *information cost* associated with the being's actions. This information cost is encapsulated in the Landauer's principle. However, before looking at the resolution, we analyse the Szilard engine—in which the being's actions allow us to convert heat into mechanical work indefinitely, without any obvious side-effects.

1.3 Szilard engine

The Szilard engine consists of a box containing a single molecule of an ideal gas, in contact with a thermal reservoir at temperature $T = 1/k_B T$, and a demon who controls a movable partition, and can measure the position of the gas molecule in the box [1].

Let's say the box has length *L*, uniform cross-section area *A*, and volume V = AL. The thermodynamic cycle involved in the Szilard engine, consists of the following four steps [5]:

- 1. Insertion of the partition The demon inserts the partition at position l (0 < l < L) reversibly and quasistatically. Let r denote the position of the molecule, with r = 0 meaning that the molecule is to the left of the partition, and r = 1 meaning that the molecule is to the right of the partition. If we put x = l/L, the probability that the particle is found to the left is P(r = 0) = x and the probability that the particle is found to the right is P(r = 1) = 1 - x.
- 2. Measurement The demon measures the position of the particle.

3. Feedback The gas is expands quasistatically and isothermally. Since this process is quasistatic, the work extracted is equal to the change in free energy,

$$W = \Delta F = \frac{1}{\beta} \ln \frac{Z(X_2)}{Z(X_1)} = \frac{1}{\beta} \ln \frac{X_2}{X_1},$$
(1.14)

where *X* is the position of the partition, X_1 being the initial position and the X_2 being the final position; Z(X) is the partition function of the single molecule gas when the partition is at *X*, and is proportional to X^1 . If $W^{(0)}$ and $W^{(1)}$ denote the work done when the molecule is found to the left and right respectively, we have

$$\beta W^{(0)} = -\ln(x); \quad \beta W^{(1)} = -\ln(1-x) \tag{1.15}$$

4. Removal of the partition The demon removes the partition quasistatically and the engine returns to its initial state.

The average work extracted in one such cycle is given by

$$\beta \langle W \rangle = \beta \sum_{r} P(r) W^{(r)} = -x \ln(x) - (1-x) \ln(1-x).$$
(1.16)

We note that when the partition is placed in the middle, i.e. x = 1/2, the amount of work extracted is $k_B T \ln 2$.

1.3.1 Measurement errors

In this section, we will spend some time analysing the case when the measurement in *Step 2* of the cycle is not perfect [5].

The magnitude of error is contained in the conditional probabilities P(q|r)—the probability that the measurement outcome² is q, when the actual position of the molecule is r. In terms of conditional probabilities, the error rate is e = P(0|1) = P(1|0).

After making the measurement, the state of the system has to be described by the pair (r,q). For example, if the measurement yields q = 1 in presence of errors, r may not be 1; the state r = 0 has probability P(1|0) = e, and the state r = 1 has probability P(1|1) = 1-e.

Hence, after measurement the system occupies one of the four states in Table 1.1.

We assume that after the expansion, the partition moves to position $x_0^{eq} = l_0^{eq}/L$ when q = 0, and to $x_1^{eq} = l_1^{eq}/L$ when q = 1. If the work from a particular configuration (r,q) of the system is denoted by $W^{(r,q)}$, we have

$$\beta W^{(1,1)} = \log\left(\frac{x_1^{eq}}{x}\right); \quad \beta W^{(1,0)} = \log\left(\frac{x_0^{eq}}{x}\right);$$
$$\beta W^{(0,1)} = \log\left(\frac{1 - x_1^{eq}}{1 - x}\right); \quad \beta W^{(0,0)} = \log\left(\frac{1 - x_0^{eq}}{1 - x}\right). \tag{1.17}$$

The average work extracted in the entire process is given by

$$\beta \langle W \rangle = -x \log x - (1 - x) \log(1 - x) + (1 - e) [x \log x_1^{eq} + (1 - x) \log(1 - x_0^{eq})] + e [x \log x_0^{eq} + (1 - x) \log(1 - x_1^{eq})].$$
(1.18)

¹Partition function for a classical ideal gas is given by $Z(T, N, V) = \frac{1}{N!} \left(\frac{V}{\lambda(T)}\right)^N$, and $X \propto V$.

Table 1.1: States available to the single particle SZE

r q	r = 0	r = 1
q = 0 $q = 1$	(0, 0) (0, 1)	(1, 0) (1, 1)

 $^{^{2}}q = 0$ means that the molecule is to the left, q = 1 means that the molecule is to the right



Figure 1.1: Work output from a single particle Szilard engine with errors.

In order to determine x_0^{eq} and x_1^{eq} , $\langle W \rangle$ is maximized by setting $\partial \langle W \rangle / \partial x_0^{eq} = 0$ and $\partial \langle W \rangle / \partial x_1^{eq} = 0$, which gives

$$x_0^{eq} = \frac{x(1-e)}{(1-e)x + (1-x)e}$$
(1.19)

$$x_1^{eq} = \frac{(1-x)(1-e)}{(1-x)(1-e) + xe}.$$
(1.20)

1.3.2 Multi-particle Szilard engine

It is possible to generalise the results in this section to the case of multiple particle with only minimal effort.

We consider a box containing *N* molecules as working substance contained in a box of volume V = AL. In the first step, the partition is placed at a position *l* which divides the box in ratio x : 1 - x with x = l/L. In the second step, the number of molecules to the left of the partition are measured: let's say that *m* molecules are found on the left and N - m molecules are found on the right side of the partition. In the third step, the gas expands isothermally till the equilibrium position $x_m^{eq} = l_m^{eq}/L$ —determined by the force balance condition—is attained. In the final step, the partition is removed and the engine is returned to its initial state.

For the average work done during one cycle of the engine, we invoke (2.13)

$$\langle W \rangle = -\frac{1}{\beta} \sum_{m=0}^{N} f_m \ln\left(\frac{f_m}{f_m^*}\right), \qquad (1.21)$$

where

$$f_m = \frac{Z_{m,N-m}(l)}{\sum_{n=0}^{N} Z_{n,N-n}(l)},$$
(1.22)

with $Z_{m,N-m}(X) = Z_m(X)Z_{N-m}(L-X)$, is interpreted as the probability that *m* molecules are found on the left side of the partition after its insertion, and

$$f_m^* = \frac{Z_{m,N-m}(l_m^{eq})}{\sum_{n=0}^N Z_{n,N-n}(l_m^{eq})}$$
(1.23)

is interpreted as the probability that m molecules are found on the left side of the partition when it is inserted at l_m^{eq} in the time backward process.



Figure 1.2: Work output from a multi particle Szilard engine parametrised by number of particles.

In case of a system of classical particles, we have $Z_m(X) = cX^m/m!$ and

$$f_{m} = \frac{Z_{m}(l)Z_{N-m}(L-l)}{\sum_{n} Z_{n}(l)Z_{N-m}(L-l)}$$

$$= \frac{l^{m}}{m!} \frac{(L-l)^{N-m}}{(N-m)!} / \sum_{n=0}^{N} \frac{l^{n}}{n!} \frac{(L-l)^{N-n}}{(N-n)!}$$

$$= \binom{N}{m} \frac{l^{m}[L-l]^{N-m}}{L^{N}}$$

$$= \binom{N}{m} x^{m} (1-x)^{N-m}.$$
(1.24)

Similarly if we let $l_m^{eq} = (m/N)L = \alpha L$, we get

$$f_m^* = \binom{N}{m} \alpha^m (1 - \alpha)^{N - m}.$$
(1.25)

Using these expressions for f_m , and f_m^* in (1.21) leads us to the following relation for work extracted

$$\beta \langle W \rangle = -\sum_{m=0}^{N} {N \choose m} x^m (1-x)^{N-m} \ln\left[\left(\frac{x}{\alpha}\right)^m \left(\frac{1-x}{1-\alpha}\right)^{N-m}\right].$$
(1.26)

1.4 Landauer's principle

The cycle involved in the operation of the Szilard engine seems to show us a process whose sole outcome is the complete conversion of heat to work, in contradiction to the second law of thermodynamics. As already noted, this contradiction is resolved by considering the combined engine–demon system, and associating an energy cost to the demon's actions. This energy cost manifests itself in Landauer's principle, which states that *the erasure of an unknown bit of information requires dissipation of at least* $k_B T \ln 2$ *of energy*.

In what follows, we shall consider the Szilard engine with a single particle in which the partition is inserted symmetrically in the first step, for simplicity.

After the measurement in *Step 2* of the Szilard engine cycle, the demon acquires one bit of information: when the molecule is to the left of the barrier, the bit value is 0, and when the molecule is to the right of the barrier, the bit value is 1. If the process is to be cyclic, the state of the demon's memory must be reset. Hence, the work per cycle of the Szilard engine is

$$W_{tot} = W + W_{eras} \ge -k_B T \ln 2 + k_B T \ln 2 = 0, \qquad (1.27)$$

where we invoked Landauer's principle to obtain a bound for the work done in bit erasure $W_{eras} \ge k_B \ln 2$.

Landauer's principle can be illustrated if as a *memory device* we have Szilard's box divided into two equal volumes with the bit encoded as the half volume containing the molecule. Our task is to reset the state of the memory device to 0. This can be achieved by first removing the partition, which destroys the bit value, and then by inserting a new partition at the right end and (isothermally) moving it to the middle of the box. The isothermal expansion of the single molecule gas involves the amount of work

$$W_{eras} = k_B T \int_{V}^{V/2} p dV = k_B T \ln 2.$$
 (1.28)

1.5 Outline of the project

Having looked at the links between the theory of information and thermodynamics which are manifest in the Szilard engine and Landauer's principle, we pursue this thread further, and look at a completely quantum description of a multi-particle Szilard engine [3] in *Chapter 2*. The quantum Szilard engine presents some intriguing differences from the classical case: insertion of partition cannot be done without expenditure of work, and when there are two or more particles, different particle statistics lead to dramatically different work outputs for bosons and fermions.

In *Chapter 3* we look at more general quantum thermodynamic cycles. We follow the development of quantum thermodynamics in [6] and [7] and define the quantum analogues of isothermal, adiabatic, isochoric, and isobaric processes. Using these quantum thermodynamic processes, quantum versions of the Carnot, Otto, Brayton, and Diesel cycles are built and their work output, efficiencies, and positive work conditions derived, when the working substance is a single-mode radiation field in a cavity.

Finally, in *Chapter 4* we look at a proof-of-concept, magnetically driven quantum heat engine with a particle trapped in a cylindrical potential well as the working substance [4]. The thermodynamic processes are driven by quasistatically modifying an external magnetic field, which modifies the confinement length of the particle. In addition to the Carnot cycle, an *isoenergetic cycle* is also described; work output and efficiencies are calculated for each of the cycles and the results compared to the expressions obtained by more general considerations in [6].

2 Quantum Szilard Engine

The most primitive construction of a Szilard engine involves a single molecule of gas—a quantum object as working substance and therefore needs a quantum description. In this chapter, we shall look at the complete quantum analysis of a multi-particle Szilard engine that has been carried out in [3]. Interestingly, we note that this came relatively recently in 2011, even though the Szilard engine has been around for a hundred years.

2.1 Quantum first law of thermodynamics

For a system with single particle states $|n\rangle$ described by $\hat{H} |n\rangle = E_n |n\rangle$, the internal energy of the system is identified as the ensemble average of the Hamiltonian

$$U = \sum_{n} P_{n} E_{n}, \qquad (2.1)$$

where P_n is the mean occupation number of the *n*th eigenstate. Taking the exterior derivative of (2.1) gives us

$$dU = \sum_{n} (E_n dP_n + P_n dE_n), \qquad (2.2)$$

which we identify as the quantum analogue of the first law: dU = dQ + dW. As dQ = T dS and $S = k_B \sum_n P_n \ln P_n$, we identify

$$dQ = \sum_{n} E_n dP_n$$
 and $dW = \sum_{n} P_n dE_n$. (2.3)

In an isothermal process the system is kept in equilibrium with a heat reservoir at temperature $T = 1/k_B\beta$, and the occupation probabilities satisfy the canonical distribution

$$P_n = \frac{e^{-\beta E_n}}{Z(\beta)},\tag{2.4}$$

where *Z* is the partition function. If an external parameter *X* (on which E_n and P_n depend smoothly) changes from X_1 to X_2 , the work is obtained from the change in free energy

$$W = \Delta F = k_B T \int_{X_1}^{X_2} \frac{\partial \ln Z}{\partial X} dX$$
(2.5)

$$= k_B T [\ln Z(X_2) - \ln Z(X_1)].$$
(2.6)

In the next section, we shall look at the work done in each of the steps of the thermodynamic cycle of the Szilard engine.

2.2 Szilard engine cycle

1. Insertion of partition A wall is isothermally inserted at position *l*. The partition function when the wall has been inserted but the measurement is not performed yet is $Z(l) = \sum_{m=0}^{N} z_m(l)$,

where $z_m(l) = Z_m(l)Z_{N-m}(L-l)$ is the partition function for the case in which *m* particles are on the left and N - m particles on the right. The amount of work expended in the insertion is given by

$$W_{ins} = k_B T [\ln Z(l) - \ln Z(L)].$$
(2.7)

- 2. Measurement Measurement is performed without any expenditure of work.
- 3. Isothermal expansion Work due to the isothermal expansion when *m* particles are to the left of the wall and N m are to the right is given by

$$W_{exp}^{(m)} = k_B T [\ln z_m(l_{eq}^m) - \ln z_m(l)], \qquad (2.8)$$

as the partition moves from the initial position *l*, to equilibrium position l_{eq}^m . Equilibrium position is determined by the force balance condition $F^{right} + F^{left} = 0$. Work is averaged over the number of particles *m* to give

$$W_{exp} = \sum_{m=0}^{N} f_m W_{exp}^{(m)} = k_B T \sum_{m=0}^{N} f_m [\ln z_m (l_{eq}^m) - \ln z_m (l)]$$
(2.9)

where $f_m = z_m(l)/Z(l)$ is the probability of finding *m* particles on the left at measurement.

4. Removal of partition During the expansion process, the barrier height due to the wall is considered to be large enough that the tunnelling time τ_t between two sides is much larger than the operational time of the thermodynamic process τ . During wall removal however, τ_t becomes comparable to τ for a certain barrier height X_0 ; beyond this barrier height the eigenstates are delocalised over both sides due to tunnelling. When the eigenstates are delocalised, the partition function is given by $Z(l_{eq}^m) = \sum_n z_n(l_{eq}^m)$ rather than $z_m(l_{eq}^m)$. The work (when *m* particles are to the left) is then given by

$$W_{rem}^{(m)} = k_B T \left[\int_{X_{\infty}}^{X_0} \frac{\partial \ln z_m(l_{eq}^m)}{\partial X} dX + \int_{X_0}^0 \frac{\partial \ln Z(l_{eq}^m)}{\partial X} dX \right]$$
(2.10)

For quasistatic processes, $\tau \to \infty$ ($X_0, X_\infty \to \infty$), and the first term above vanishes and

$$W_{rem}^{(m)} = k_B T \int_{X_0}^0 \frac{\partial \ln Z(l_{eq}^m)}{\partial X} dX = k_B T [\ln Z(L) - \ln Z(l_{eq}^m)]$$
(2.11)

This work is averaged over all m to give

$$W_{rem} = k_B T \sum_{m=0}^{N} f_m [\ln Z(L) - \ln Z(l_{eq}^m)].$$
(2.12)

Combining contributions from all four steps of the engine cycle, the total work in a cycle is given by

$$W_{tot} = W_{ins} + W_{exp} + W_{rem} = -k_B T \sum_{m=0}^{N} f_m \ln\left(\frac{f_m}{f_m^*}\right)$$
(2.13)

where $f_m^* = z_m (l_{eq}^m)/Z(l_{eq}^m)$ is identified with the probability of obtaining *m* particles on the left in the time backward process when the partition is inserted at l_{eq}^m .

2.3 Single particle quantum Szilard engine

We consider a single particle in an infinite square well of size *L* and we assume that the partition is inserted at position l = L/2 for simplicity. Since the partition is inserted in the middle of the well, $f_0 = f_1 = 1/2$. In this case, the partition moves to an end of the partition during expansion, hence $Z(l_{eq}^m) = z_m(l_{eq}^m)$ and therefore $f_0^* = f_1^* = 1$. The total work done is obtained from a straightforward application of (2.13)

$$W_{tot} = k_B T \ln 2.$$
 (2.14)

It is observed that the work done from the quantum version of the single particle Szilard engine is identical to the work obtained from its classical counterpart.

In order to highlight differences between the quantum and the classical case, it is instructive to look at each of the processes individually.

- 1. Work done in insertion of partition $W_{ins} = -\Delta + k_B T \ln 2$ where $\Delta = \ln(z(L))/\ln(z(L/2))$, $z(l) = \sum_n e^{-\beta E_n(l)}$ is the partition function, and $E_n(l) = h^2 n^2/(8Ml^2)$ are eigenenergies with h being Planck's constant. In particular, we note the contrast from the classical case where the partition is inserted without any expenditure of work.
- 2. No work is done during the measurement, same as the classical case.
- 3. Work done during expansion $W_{exp} = \frac{\ln z(L)}{\ln z(L/2)} = \Delta$, which depends on the energy spectrum $E_n(l)$. In the classical case, the work done during expansion is $k_B T \ln 2$.
- 4. Work done in removal vanishes because $l_{eq}^m = L$, same as the classical case.

If the insertion process were ignored, $W_{tot} = \Delta$ and the second law would be violated in the low temperature limit as $\Delta \gg k_B T$.

2.4 Two particle quantum Szilard engine

In order to calculate the total work done, we look at each value of *m* in the sum of (2.13) individually. We assume that the partition is inserted at position l = L/2 in the first step. When m = 0, 2, there are no particles on one of the sides of the wall and the force balance condition leads to $l_{eq}^m = 0, L$ and therefore $f_0^* = f_1^* = 1$. When m = 1, the wall doesn't move and $l_{eq}^m = l = L/2$ which gives us $f_1 = f_1^*$. Summing all contributions, we end up with

$$W_{tot} = -2k_B T f_0 \ln f_0 \tag{2.15}$$

where we have used $f_0 = f_2$. We recall that

$$f_0 = \frac{z_0(l)}{z_0(l) + z_1(l) + z_2(l)},$$
(2.16)

and note that $z_0(l) = z_2(l)$ are the partition functions of two particles in a potential well of size l, and $z_1(l) = Z(\beta)^2$ where $Z(\beta)$ is the partition function of a single particle in a well of size l. Unless we consider the high temperature limit when the degeneracies are washed out due to thermal fluctuations, the case of bosons and fermions must be analysed separately as particle statistics come into play. However before proceeding, we record that

$$Z(\beta)^{2} = \left(\sum_{n} e^{-\beta E_{n}}\right)^{2}$$

= $\sum_{n} e^{-2\beta E_{n}} + 2\sum_{n < m} e^{-\beta(E_{n} + E_{m})},$ (2.17)

and therefore

$$\sum_{n < m} e^{-\beta(E_n + E_m)} = \frac{Z(\beta)^2 - Z(2\beta)}{2}.$$
(2.18)

2.4.1 Two bosons

When the number of particles is only two, the parity requirements on the partition sum can be satisfied with relative ease

$$z_{0} = \sum_{n \le m} e^{-\beta(E_{n} + E_{m})} = \sum_{n} e^{-2\beta E_{n}} + \sum_{n < m} e^{-\beta(E_{n} + E_{m})}$$

= $Z(2\beta) + \sum_{n < m} e^{-\beta(E_{n} + E_{m})}$
= $\frac{Z(\beta)^{2} + Z(2\beta)}{2}$, (2.19)



Figure 2.1: f_0 as a function of *T* for bosons (solid curve) and fermions (dashed curve) and classical particle (dash-dotted line). (a) Three possible ways in which two identical bosons as assigned over two states. (b) Four possible ways in which two distinguishable particles are assigned over two states. (Inset) W_{tot}/W_c as a function of temperature.

where in the last line we have used (2.18). f_0 for bosons is

$$f_0 = \frac{Z(\beta)^2 + Z(2\beta)}{4Z(\beta)^2 + 2Z(2\beta)} = \frac{d+1}{4d+1}$$
(2.20)

where $d = Z(\beta)^2 / Z(2\beta)$.

We note that $Z(\beta) > Z(2\beta)$ and hence $d = (Z(\beta)/Z(2\beta))Z(\beta) > Z(\beta)$. If the number of energy levels is infinite, in the high temperature limit, we have $Z(\beta) \to \infty$ and $d \to \infty$. Therefore, we conclude $f_0 \to 1/4$ as $T \to \infty$, which gives $W_{tot} \to k_B \ln 2$ in the high temperature limit.

If the single-particle ground state is non-degenerate, we have

$$d = \frac{1 + 2e^{-\beta(E_1 - E_0)} + \dots}{1 + 2e^{-2\beta(E_1 - E_0)} + \dots},$$
(2.21)

which gives us $d \to 1$ as $T \to 0$. Thus, in the low temperature limit, f_0 attains a limiting value $f_0 \to 1/3$, which gives $W_{tot} \to (2/3)k_BT \ln 3$.

2.4.2 Two fermions

We proceed in a manner similar to what we did for bosons. We start with calculating z_0 , the partition function of two fermions in a potential well.

$$z_0 = \sum_{n < m} e^{-\beta(E_n + E_m)} = \frac{Z(\beta)^2 - Z(2\beta)}{2}$$
(2.22)

where we have used (2.18). From here, we can write the expression for f_0 for fermions,

$$f_0 = \frac{Z(\beta)^2 - Z(2\beta)}{4Z(\beta)^2 - 2Z(2\beta)} = \frac{d-1}{4d-1}.$$
(2.23)

As in the previous section, if the number of states is infinite we obtain the high temperature limit: $f_0 \rightarrow 1/4$ and $W_{ext} \rightarrow k_B T \ln 2$; and if the single-particle ground state is non-degenerate, we have the low temperature limit: $f_0 \rightarrow 1$ and $W_{ext} \rightarrow 0$, in stark contrast to bosons.

	Bosons	Fermions
$T \rightarrow 0$	(2/3)ln3	0
$T \to \infty$	ln 2	ln 2

Table 2.1: Work done in a two particle quantum Szilard engine with l = L/2 in the low and high temperature limits in units of $k_B T$.

3 Quantum Thermodynamic Cycles

We have already identified the quantum analogues of heat, work, and the first law of thermodynamics. In this chapter we shall extend some common thermodynamic cycles to quantum systems and then describe quantum analogues of classical heat engine cycles: Carnot, Otto, Brayton, and Diesel. We derive work output, efficiency, and positive work condition (PWC) for these quantum heat engine cycles and compare with their classical counterparts.

Finally, for an illustration of concepts developed, we shall look at quantum heat engines based on a single-mode radiation field in a cavity.

3.1 Quantum thermodynamic processes

Before starting with the description of quantum thermodynamic processes, we stop to record a fact that will make certain computations easier: the work done dW, heat exchanged dQ, and therefore the change in internal energy dU, are invariant under a uniform shift of all energy levels.

If we assume that all energy levels shift uniformly: $E'_n = E_n + \delta$, the first thing we note is that that $dE'_n = dE_n$ because δ is a constant. Next, we consider the occupation probabilities,

$$P'_{n} = e^{-\beta(E_{n}+\delta)} \left(\sum_{m} e^{-\beta(E_{m}+\delta)}\right)^{-1} = e^{-\beta E_{n}} \left(\sum_{m} e^{-\beta E_{m}}\right)^{-1} = P_{n},$$
(3.1)

and observe that $dP'_n = dP_n$. Finally, from the quantum analogues of heat, work (2.3); and the first law (2.2), the result follows.

In particular we note that, assuming ground state energy to be zero has no effect on dU.

3.1.1 Isothermal process

When the working substance is in equilibrium with a heat bath, its temperature is well defined and is equal to the temperature of the bath. Specifically, for a two-level system in equilibrium with a bath, with states $|g\rangle$ and $|e\rangle$, and energy spacing $\Delta = E_e - E_g$, the occupation probabilities P_g and P_e must satisfy the canonical distribution:

$$P_g = \frac{e^{-\beta E_g}}{Z(\beta)}; \quad P_e = \frac{e^{-\beta E_e}}{Z(\beta)}, \tag{3.2}$$

where $Z(\beta) = e^{-\beta E_s} + e^{-\beta E_e}$ is the partition function of the two-level system. These relations lead to

$$\frac{P_e}{P_g} = e^{-\beta\Delta}.$$
(3.3)

Even when the working substance is not in equilibrium with a heat bath we can define an *effective temperature* by inverting (3.3)

$$T_{eff} = \frac{1}{k_B \beta_{eff}} = \frac{\Delta}{k_B} \left(\ln \frac{P_g}{P_e} \right)^{-1}.$$
(3.4)

In particular, we note that the effective temperature is well defined for all two-level systems. For more than two levels, the occupation probabilities must satisfy the canonical distribution for a unique T_{eff} to be defined.

In a quantum isothermal process, the working substance is confined to a potential energy well, kept in contact with a heat bath, and occupation probabilities P_n and energy levels E_n change simultaneously, so that the occupation probabilities satisfy the canonical distribution (2.4) for a fixed β at all times.

Internal energy in an isothermal process When the working substance is a classical ideal gas, the internal energy remains invariant in an isothermal process. However, this classical result changes when the working substance is a quantum system. In particular, we note that quantum isoenergetic process cannot be considered the quantum analogue of the isothermal process.

The internal energy of a system is $U(i) = \langle H \rangle = \sum_n E_n P_n$. In an isothermal expansion process, all energy levels change in the same ratio $E_n \rightarrow \zeta E_n$, n = 0, 1, 2, ..., where $\zeta > 0$ is the ratio of energy levels. The internal energy of the system can be rewritten as

$$U(\zeta) = \sum_{n} \frac{\zeta E_n}{Z(\zeta)} e^{-\beta \zeta E_n}.$$
(3.5)

We now consider the derivative of the internal energy with respect to ζ ,

$$\frac{\mathrm{d}U(\zeta)}{\mathrm{d}\zeta} = \sum_{n} \frac{E_{n}}{Z(\zeta)} (1 - \zeta\beta E_{n}) e^{-\beta\zeta E_{n}} + \zeta\beta \left(\sum_{n} \frac{E_{n}}{Z(\zeta)} e^{-\beta\zeta E_{n}}\right)^{2}$$
(3.6)

For two-level systems in particular, there is only one term in the sum (because we can assume the ground state energy to be zero without loss of generality), and we have

$$\frac{\mathrm{d}U(\zeta)}{\mathrm{d}\zeta} = \frac{E_e}{Z(\zeta)} e^{-\beta\zeta E_e} \left(1 - \frac{\zeta\beta E_e}{Z(\zeta)}\right),\tag{3.7}$$

which is non-zero. Hence, the internal energy is not invariant in this isothermal process.

3.1.2 Isochoric process

In a quantum isochoric process no work is done while heat is exchanged between the working substance and the heat bath. Energy spectrum remains fixed, while the occupation probabilities change until the working substance reaches an equilibrium with the bath.

3.1.3 Adiabatic process

In a quantum adiabatic process, the time evolution of the system is controlled by slowly changing parameters For such a Hamiltonian, transitions between different eigenstates $|n\rangle \rightarrow |m\rangle$ are forbidden, and the occupation probabilities remain invariant.

From our earlier discussion $dP_n = 0 \implies dQ = 0$. Hence, a quantum adiabatic process is thermodynamic adiabatic. However the converse may not always be true: if a classical adiabatic process proceeds very fast, the quantum adiabatic condition will not be satisfied and internal excitations might occur.

3.1.4 Isobaric process

From classical thermodynamics, we know that $dW = \sum_i Y_i dy_i$, where Y_i are generalised forces and y_i are generalised displacements with

$$Y_n = \frac{\mathrm{d}W}{\mathrm{d}y_n}.\tag{3.8}$$

When the generalized displacement is chosen to be volume, the conjugate force is pressure P = -dW/dV. Motivated by the definition of a generalized force in a classical system, we define it for a quantum system by

$$F = -\frac{\mathrm{d}W}{\mathrm{d}L} = -\sum_{n} P_{n} \frac{\mathrm{d}E_{n}}{\mathrm{d}L},\tag{3.9}$$

with F and L being the generalized force–displacement conjugate pair. When L is a generalized coordinate of the system (for example, the width of the potential well), we identify the conjugate force as the pressure.

The quantum isobaric process is defined in the obvious way: the quantum analogue of pressure must remain invariant during the process.

3.2 Carnot cycle

Just like its classical counterpart, the quantum Carnot cycle consists of two quantum isothermal processes, and two quantum adiabatic processes (Figure 3.1). During isothermal processes, we assume that the energy levels of the system change much slower than the relaxation time of the system, and hence the system is always kept in equilibrium with the heat bath.



Figure 3.1: Temperature–entropy diagram of a Carnot engine cycle.

3.2.1 Thermodynamic reversibility

We pause here to remark about the thermodynamic reversibility of the quantum Carnot cycle. In order to ensure that the cycle is reversible, the following two conditions must be satisfied by the quantum adiabatic process:

- (1) After the quantum adiabatic process $(B \rightarrow C)$, we can use an effective temperature T_C to characterize the working substance
- (2) The effective temperature T_C of the working substance, after the quantum adiabatic process equals the temperature T_C of the heat bath of the following isothermal process $(C \rightarrow D)$.

If either of the two conditions are not satisfied, a thermalisation process is inevitable before the succeeding isothermal process starts, which renders the cycle irreversible. It can be shown [6] that the these conditions are equivalent to the following two conditions

(a) All energy gaps are changed by the same ratio in the quantum adiabatic process

$$\frac{E_n(B) - E_m(B)}{E_n(C) - E_m(C)} = \lambda = \frac{E_n(A) - E_m(A)}{E_n(D) - E_m(D)}.$$
(3.10)

(b) The ratio of change in energy gaps in the adiabatic process must equal the ratio of the two temperatures of the heat bath $\lambda = T_H/T_C$.

It is easier to show the backward direction (a), (b) \implies (1), (2). Since the process $B \rightarrow C$ is adiabatic, the occupation probabilities don't change $P_n(B) = P_n(C)$; and by hypothesis, we have $E_n(B) = \lambda E_n(C)$ [where we have chosen m = 0 and $E_0(B) = E_0(C) = 0$ without any loss of generality (3.1)]:

$$P_n(B) = \frac{e^{-\beta_H E_n(B)}}{Z(\beta_H)} = \frac{e^{-\beta_H \lambda E_n(C)}}{Z(\lambda \beta_H)}$$
$$= \frac{e^{-\beta_C E_n(C)}}{Z(\beta_C)} = P_n(C), \qquad (3.11)$$

where in the second line we used $\lambda = T_H/T_C$. Hence, we have shown that at the end of the adiabatic process, the occupation probabilities satisfy a canonical distribution for temperature T_C ; the effective temperature of the working substance at *C* is well defined and it is equal to the temperature of the heat sink.

For the forward direction (1), (2) \implies (a), (b), we assume that the working substance is in equilibrium with the heat bath at T_H at the instant before the adiabatic process $B \rightarrow C$ starts, and the occupation probabilities satisfy

$$P_n(B) = \frac{e^{-\beta_H E_n(B)}}{Z(\beta_H)}.$$
 (3.12)

At the end of the adiabatic process the working substance is characterised by the effective temperature T_c . Since the occupation probabilities remain unchanged during the process we have

$$\frac{P_n(B)}{P_m(B)} = \frac{e^{-\beta_H E_n(B)}}{e^{-\beta_H E_m(B)}} = \frac{P_n(C)}{P_m(C)} = \frac{e^{-\beta_C E_n(B)}}{e^{-\beta_C E_m(B)}},$$
(3.13)

which implies

$$E_n(C) - E_m(C) = \frac{T_C}{T_H} [E_n(B) - E_m(B)], \qquad (3.14)$$

which is a combination of conditions (1) and (2).

3.2.2 Work and efficiency

Since the isothermal process is carried out reversibly, we can use dQ = TdS to calculate the amount of heat exchanged. The process $A \rightarrow B$ is a quantum isothermal expansion process in which heat is absorbed from the reservoir, hence $dQ = T_H dS > 0$ and

$$Q_{in}^{QIT} = T_H[S(B) - S(A)] > 0$$
(3.15)

The process $C \rightarrow D$ is a quantum isothermal compression in which heat is rejected to the reservoir, hence $-dQ = -T_C dS > 0$ and

$$Q_{out}^{QIT} = T_C[S(C) - S(D)] > 0$$
(3.16)

The entropies can be calculated from the temperature derivative of the free energy $F = -k_B T \ln Z$: $S(i) = -\partial F / \partial T$.

The work done per cycle is given by

$$W_{C} = Q_{in}^{QIT} - Q_{out}^{QIT} = (T_{H} - T_{C})[S(B) - S(A)], \qquad (3.17)$$

where we have used the relations S(B) = S(C) and S(A) = S(D), because the occupation probabilities and therefore the entropies remain invariant during adiabatic processes. Consequently, the efficiency of the quantum Carnot cycle is

$$\eta_{C} = \frac{W_{C}}{Q_{in}^{QIT}} = 1 - \frac{T_{C}}{T_{H}}$$
(3.18)

$$=1 - \frac{E_n(C) - E_m(C)}{E_n(B) - E_m(B)}$$
(3.19)

From the above relation, the *positive work condition* is $T_C < T_H$.

We note that the efficiency derived in (3.18) is identical to what we obtain for a classical Carnot cycle. In fact, the technique employed to derive the efficiency here is formally very similar to what is done for a classical Carnot cycle in *Appendix A*.

3.3 Otto cycle

The quantum Otto engine cycle consists of two quantum isochoric and two quantum adiabatic processes (Figure 3.2).



Figure 3.2: Temperature–entropy diagram of a Otto engine cycle.

3.3.1 Work and efficiency

In the isochoric process $A \rightarrow B$, no work is done, but heat is absorbed

$$Q_{in}^{QIC} = \sum_{n} \int_{A}^{B} E_{n} dP_{n} = \sum_{n} E_{n}^{H} [P_{n}(B) - P_{n}(A)].$$
(3.20)

Similarly, the heat released during the quantum isochoric cooling process $3 \rightarrow 4$, is

$$Q_{out}^{QIC} = \sum_{n} \int_{C}^{D} E_{n} dP_{n} = \sum_{n} E_{n}^{C} [P_{n}(C) - P_{n}(D)]$$
(3.21)

We cannot use dQ = TdS because the working substance and heat bath are not in thermal equilibrium during the isochoric process

In order to ensure thermodynamic reversibility of the cycle, we must require that all energy gaps change in the same ratio in the quantum adiabatic process: $E_n^H - E_m^H = \alpha [E_n^C - E_m^C]$. Occupation probabilities: $P_n(B) = P_n(C)$ and $P_n(A) = P_n(D)$ and entropies: S(B) = S(C) and S(A) = S(D) remain invariant during the adiabatic process.

Net work during one quantum Otto cycle is the difference between heat absorbed and heat rejected

$$W_{O} = Q_{in}^{QIC} - Q_{out}^{QIC} = \sum_{n} (E_{n}^{H} - E_{n}^{C}) [P_{n}(B) - P_{n}(A)]$$
(3.22)

Consequently, the operational efficiency of the Otto cycle is given by

$$\eta_O = \frac{W_O}{Q_{in}^{QIC}} = 1 - \frac{E_n^C - E_m^C}{E_n^H - E_m^H} = 1 - \frac{1}{\alpha}$$
(3.23)

3.3.2 Positive work condition

We first consider the case when the working substance has only two energy levels. The work done is given by

$$W_{O} = (E_{e}^{H} - E_{e}^{L})(P_{e}(B) - P_{e}(A))$$

= $(E_{e}^{H} - E_{e}^{L})(P_{e}^{H} - P_{e}^{L})$ (3.24)

Contribution due to the ground state vanishes because we take $E_g^L = E_g^H = 0$. As $T(A) = T_C$ and $T(B) = T_H$, the occupation probabilities obey the canonical distribution:

$$P_{e}^{H} = \frac{e^{-\beta_{H}\Delta_{H}}}{1 + e^{-\beta_{H}\Delta_{H}}}; \quad P_{e}^{L} = \frac{e^{-\beta_{L}\Delta_{L}}}{1 + e^{-\beta_{L}\Delta_{L}}}$$
(3.25)

For positive work, we take

$$W_{O} = (E_{e}^{H} - E_{e}^{L})(P_{e}^{H} - P_{e}^{L}) > 0$$

$$\Longrightarrow (P_{e}^{H} - P_{e}^{L}) > 0$$

$$\Longrightarrow \left(\frac{e^{-\beta_{H}\Delta_{H}}}{1 + e^{-\beta_{H}\Delta_{H}}} - \frac{e^{-\beta_{L}\Delta_{L}}}{1 + e^{-\beta_{L}\Delta_{L}}}\right) > 0$$

$$\Longrightarrow -\beta_{H}\Delta_{H} + \beta_{L}\Delta_{L} > 0$$

$$\Longrightarrow T_{L}\frac{\Delta_{L}}{\Delta_{H}} < T_{H}$$

$$\Longrightarrow \alpha T_{L} < T_{H}$$
(3.26)

For a multilevel Otto engine in which all energy levels change in the same ratio, the same positive work condition follows from a very similar computation, where we use the condition $\Delta_L^n = \alpha \Delta_H^n$ for all *n*. We note that the PWC for an Otto cycle ($\alpha T_L < T_H$) is stronger than the PWC for a Carnot cycle ($T_L < T_H$).

3.4 Single-mode radiation field in cavity

In this section, we shall look at illustrations of the Carnot and Otto cycles based on a single-mode radiation field in a cavity of length *L* and cross section area *A*, which supports a single-mode of field $\omega = s\pi c/L$, where *s* is an integer and *c* the speed of light. The Hamiltonian reads

$$\hat{H} = \sum_{n} \left(n + \frac{1}{2} \right) \hbar \omega \left| n \right\rangle \langle n |, \qquad (3.27)$$

where $|n\rangle$ is the Fock state of the radiation field. In heat engines based on single-mode radiation, the quantum thermodynamic processes are controlled by (quasistatically and reversibly) varying the length of the cavity *L*, which in turn changes the frequency of allowed modes ω . In what follows, we shall use ω and *L* as stand-ins for each other.

Energy spectrum of the system is $E_n = \hbar \omega (n + 1/2)$ and the partition function is evaluated

$$Z(\beta,\omega) = \sum_{n} e^{-\beta E_{n}} = e^{-\beta \hbar \omega/2} \sum_{n} e^{-n\beta \hbar \omega}$$
$$= \frac{e^{-\beta \hbar \omega/2}}{1 - e^{\beta \hbar \omega}} = \left[2 \sinh\left(\frac{\beta \hbar \omega}{2}\right) \right]^{-1}.$$
(3.28)

The ensemble average energy can be evaluated with $(\partial \ln Z / \partial \beta)$:

$$U(\beta,\omega) = \frac{\partial \log Z}{\partial \beta} = \frac{1}{Z} \frac{\partial Z}{\partial \beta}$$
$$= \frac{1}{Z} \left(\frac{\hbar \omega}{2} \frac{\coth(\beta \hbar \omega/2)}{2\sinh(\beta \hbar \omega/2)} \right)$$
$$= \frac{\hbar \omega}{2} \coth\left(\frac{\beta \hbar \omega}{2}\right)$$
(3.29)
$$= \left[\frac{1}{e^{\beta \hbar \omega} - 1} + \frac{1}{2} \right] \hbar \omega$$
(3.30)

and the entropy with the negative of the *T* derivative of the free energy $F = -k_B T \ln Z$

$$S(\beta, \omega(i)) = k_B \frac{\partial T \ln Z}{\partial T} = k_B \left(\ln Z + T \frac{\partial \ln Z}{\partial \beta} \frac{\partial \beta}{\partial T} \right)$$
$$= k_B (\ln Z - \beta U)$$
(3.31)

$$= -k_B \ln\left[2\sinh\left(\frac{\beta\hbar\omega(i)}{2}\right)\right] - k_B \frac{\beta\hbar\omega(i)}{2} \coth\left(\frac{\beta\hbar\omega(i)}{2}\right).$$
(3.32)

Before calculating the quantum analogue of pressure (radiation force), we note that the adiabatic (isoentropic) condition for this system is $\beta \omega$ = constant or equivalently

$$TL = \text{constant.}$$
 (3.33)

Radiation force We begin by noting that $dE_n/dL = -E_n(L)/L$, and calculate the radiation force *F* as a function of temperature and cavity length from (3.9). For this calculation we assume that the system is in equilibrium with a heat bath at temperature $T = 1/k_B\beta$ and the occupation probabilities satisfy the canonical distribution,

$$F = -\sum_{n} \frac{e^{-\beta E_n(L)}}{Z(L)} \frac{\mathrm{d}E_n(L)}{\mathrm{d}L} = \frac{1}{LZ(L)} \sum_{n} e^{-\beta E_n(L)} E_n(L)$$
$$= \frac{1}{L} \left[-\frac{1}{Z(L)} \frac{\partial Z(L)}{\partial \beta} \right] = \frac{\hbar s \pi c}{L^2} \left[\frac{1}{e^{\beta \hbar s \pi c/L} - 1} + \frac{1}{2} \right]$$
(3.34)

$$=\frac{1}{L}\left[\frac{1}{e^{\beta\hbar\omega}-1}+\frac{1}{2}\right]\hbar\omega.$$
(3.35)

We identify (3.34) with the equation of state for this system. In particular, for an isobaric process, the temperature must be varied in the following very subtle way:

$$\beta = \frac{L}{\hbar s \pi c} \ln \left(\frac{2FL^2 + \hbar s \pi c}{2FL^2 - \hbar s \pi c} \right), \tag{3.36}$$

from which we derive another equivalent condition for the adiabatic process

$$FL^2 = \text{constant.}$$
 (3.37)

3.4.1 Carnot cycle

Work done in a Carnot cycle can be calculated from (3.17)

$$W_C = (T_H - T_C)[S(B) - S(A)], \qquad (3.38)$$

where *S*(*B*) and *S*(*C*) depend on the size of the cavity $L(i) = s\pi c/\omega(i)$, and are calculated from (3.32).

3.4.2 Otto cycle

Work done in the Otto cycle is calculated from (3.22)

$$W_O^{HO} = \sum_n (E_n^H - E_n^C)(P_n^H - P_n^C)$$

= $\hbar(\omega_H - \omega_C) \sum_n \left(n + \frac{1}{2}\right)(P_n^H - P_n^C)$
= $\hbar(\omega_H - \omega_C)(\langle n \rangle^H - \langle n \rangle^C),$ (3.39)

where $\langle n \rangle^i = [e^{\beta \hbar \omega(i)} - 1]^{-1}$ is the mean photon number at a particular stage in the cycle.



Figure 3.3: Force-displacement diagram of a Brayton cycle. $A \rightarrow B$ represents isobaric expansion with a constant force; $B \rightarrow C$ represents an adiabatic expansion with constant entropy; $C \rightarrow D$ represents an isobaric compression with a constant force; $D \rightarrow A$ is another adiabatic compression with constant entropy

3.5 Brayton cycle

Having looked at the thermodynamics of the single-mode radiation, and deriving the quantum equivalent of pressure in the system we shall look at the quantum Brayton cycle in this section.

Brayton cycle is illustrated in Figure 3.3. We note that the quantum adiabatic processes in the cycle must satisfy these extra conditions to ensure reversibility:

- 1. All energy level spacings of the working substance change in the same ratio
- 2. This ratio is equal to the ratio of temperatures of the two heat baths just before and after the adiabatic process

These conditions are very similar to the ones we needed for ensuring the reversibility of the Carnot cycle; and are satisfied by the single-mode radiation.

3.5.1 Work and efficiency

We calculate the work done in a Brayton cycle based on single-mode radiation. Heat absorbed in the isobaric expansion process $A \rightarrow B$ is given by

$$Q_{A\to B} = \int_{A}^{B} \left[\sum_{n} E_{n}(L) \frac{\mathrm{d}P_{n}(L)}{\mathrm{d}L} \right] \mathrm{d}L$$

= $[U(L_{B}) - U(L_{A})] + \int_{A}^{B} F(L) \mathrm{d}L$
= $[F(L_{B})L_{B} - F(L_{A})L_{A}] + F_{1}(L_{B} - L_{A})$
= $2F_{1}(L_{B} - L_{A}),$ (3.40)

where we have used U(L) = LF(L) due to (3.34). Similarly, heat released in the isobaric compression process $C \rightarrow D$ is

$$Q_{C \to D} = 2F_0(L_C - L_D). \tag{3.41}$$

Since no heat is exchanged in the adiabatic processes, work extracted during the cycle is

$$W = Q_{A \to B} - Q_{C \to D}$$

= 2[F₁(L_B - L_A) - F₀(L_C - L_D)], (3.42)

and the efficiency is given by

$$\eta_B = 1 - \frac{F_0(L_C - L_D)}{F_1(L_B - L_A)}.$$
(3.43)

Due to the adiabatic condition (3.37), we have $F_1/F_0 = (L_C/L_B)^2 = (L_D/L_A)^2$, which can be used to simplify the efficiency to

$$\eta_B = 1 - \left[\frac{F_0}{F_1}\right]^{1/2}.$$
(3.44)

Positive work condition deduced from the above expression is $F_0 < F_1$.

3.6 Diesel cycle

The Diesel cycle is illustrated in Figure 3.4; it consists of an isobaric, two adiabatic, and an isochoric process. As before, in order to ensure reversibility, all energy-level spacings must change in the same ratio in the adiabatic processes [6].



Figure 3.4: Force-displacement diagram of a Diesel engine cycle. $A \rightarrow B$ represents isobaric expansion with a constant force; $B \rightarrow C$ represents an adiabatic expansion with constant entropy; $C \rightarrow D$ represents an isochoric compression with constant volume; $D \rightarrow A$ is another adiabatic compression with constant entropy.

3.6.1 Work and efficiency

In order to calculate the work and efficiency, we employ the now familiar standard procedure to calculate heat absorbed and rejected during the cycle. Heat is absorbed in the isobaric process $A \rightarrow B$, and it is the same as in (3.40)

$$Q_{A \to B} = 2F_1(L_B - L_A). \tag{3.45}$$

Heat rejected in the isochoric process $C \rightarrow D$ equals the change in internal energy

$$Q_{C \to D} = U(C) - U(D)$$

= $L_1(F_C - F_D),$ (3.46)

where we have used FL = U due to (3.30), and $L_C = L_D = L_1$ to go to the second step. Work done is the difference between heat absorbed and heat rejected:

$$W_{D} = 2F_{1}(L_{B} - L_{A}) - L_{1}(F_{C} - F_{D})$$

$$= F_{1}L_{1}\left[2\left(\frac{L_{B}}{L_{1}} - \frac{L_{A}}{L_{1}}\right) - \left(\frac{F_{C}}{F_{1}} - \frac{F_{D}}{F_{1}}\right)\right]$$

$$= F_{1}L_{1}(r_{E} - r_{C})[2(r_{E} + r_{C}) - 1], \qquad (3.47)$$

where we have defined the expansion coefficient $r_E = L_B/L_1$, the compression coefficient $r_C = L_A/L_1$, and used the adiabatic condition $FL^2 = \text{constant}$. The efficiency is given by

$$\eta_D = 1 - \frac{1}{2} (r_E - r_C). \tag{3.48}$$

Positive work condition deduced from the above expression is $2 + r_C > r_E$.

4 Magnetically Driven Quantum Heat Engine

In this chapter we shall look at a proof-of-concept quantum heat engine based on a quantum dot and driven by an external magnetic field [4].

4.1 Single particle spectrum in a cylindrical well

As working substance, we consider a single particle confined in a cylindrical potential of the form

$$V_{dot}(x,y) = \frac{1}{2}m^*\omega_d(x^2 + y^2),$$
(4.1)

where m^* is the effective mass of the particle. In addition to this, we apply a traverse magnetic field $\mathbf{B} = B\hat{z}$ for additional confinement. This field is generated by a vector potential, for which we adopt the symmetric gauge

$$\mathbf{A} = \frac{B}{2}(-y\hat{x} + x\hat{y}) \tag{4.2}$$

The Hamiltonian for a particle in geometric confinement V_{dot} and vector potential **A** has the form

$$\hat{H} = \frac{1}{2m^*} \left[\left(p_x - \frac{eBy}{2} \right) + \left(p_y + \frac{eBx}{2} \right) \right] + V_{dot}(x, y),$$
(4.3)

and solving the eigenvalue equation $\hat{H} |\psi\rangle = E |\psi\rangle$ gives the following energy spectrum [8]:

$$E_{n_{\rho},m} = \hbar\Omega[2n_{\rho} + |m| + 1] + m\frac{\hbar\omega_{B}}{2},$$
(4.4)

which are energies corresponding to *effective Landau levels* $|n_{\rho}, m\rangle$, where $n_{\rho} = 0, 1, 2, ...$ and $m = 0, \pm 1, \pm 2, ...$ are the radial and azimuthal quantum numbers respectively, $\omega_B = eB/m^*$ is the cyclotron frequency, and we call $\Omega = [\omega_d^2 + \omega_B^2/4]^{1/2}$ the effective frequency. We note that the energy eigenfunctions are associated Laguerre polynomials [8]

$$\langle \mathbf{r} | \psi_{n_{\rho},m} \rangle \sim e^{-\rho^2/2l_{e,B}} L_{n_{\rho}}^{|m|} (\rho^2/l_{e,B}^2).$$
 (4.5)

Effective Landau radius is defined as

$$l_{e,B} = \left[\frac{\hbar}{m^*\Omega}\right]^{1/2},\tag{4.6}$$

is the characteristic length of the system, and has contributions from the geometric confinement $l_d = [\hbar/m^*\omega_d]^{1/2}$ and confinement due to the magnetic field $l_B = [\hbar/m^*\omega_B]^{1/2}$:

$$l_{e,B} = \left[\frac{1}{l_d^4} + \frac{1}{4l_B^4}\right]^{-1/4}.$$
(4.7)

4.2 Quantum dot thermodynamics

Before going on to look at the heat engine cycles, we pause to record some thermodynamic facts about the system in question. We shall first evaluate the partition function for a single particle, and then derive expressions for entropy and ensemble average energy.



Figure 4.1: Single particle energy spectrum as a function of applied magnetic field.

4.2.1 Single particle partition function

For calculating the partition function, it is convenient to parametrize the energy in terms of quantum numbers $n_{\pm} = 0, 1, 2, ...$ such that

$$n_{\pm} = \frac{1}{2} [2n_{\rho} + |m| \pm m]$$
(4.8)

and $2n_{\rho} + |m| = n_{+} + n_{-}$ and $m = n_{-} - n_{+}$, in terms of which the energy is written

$$E_{\mathbf{n}} = \hbar\Omega[2n_{\rho} + |m| + 1] + m\frac{\hbar\omega_{B}}{2}$$

$$= \hbar\left[\Omega + \frac{\omega_{B}}{2}\right]n_{+} + \hbar\left[\Omega - \frac{\omega_{B}}{2}\right]n_{-} + \hbar\Omega$$

$$= \hbar\omega_{+}\left[n_{+} + \frac{1}{2}\right] + \hbar\omega_{-}\left[n_{-} + \frac{1}{2}\right]$$

$$= E(n_{+}) + E(n_{-}), \qquad (4.9)$$

where we identify $\omega_{\pm} = \Omega \pm \omega_B/2$.

It is now easy to carry out the partition sum,

$$Z(\beta) = \sum_{n_{+}} e^{-\beta E(n_{+})} \sum_{n_{-}} e^{-\beta E(n_{-})}$$
$$= \left[e^{\beta \hbar \omega_{+}/2} \sum_{n_{+}} e^{-n_{+}\beta \hbar \omega_{+}} \right] \left[e^{\beta \hbar \omega_{-}/2} \sum_{n_{-}} e^{-n_{-}\beta \hbar \omega_{-}} \right]$$
$$= \left[2 \sinh\left(\frac{\beta \hbar \omega_{+}}{2}\right) \right]^{-1} \left[2 \sinh\left(\frac{\beta \hbar \omega_{-}}{2}\right) \right]^{-1}.$$
(4.10)

4.2.2 Ensemble average energy and entropy

The ensemble average energy is calculated with $U = -\partial \ln Z / \partial \beta$

$$U = \frac{\hbar\omega_{+}}{2} \operatorname{coth}\left(\frac{\beta\hbar\omega_{+}}{2}\right) + \frac{\hbar\omega_{-}}{2} \operatorname{coth}\left(\frac{\beta\hbar\omega_{-}}{2}\right).$$
(4.11)

And the entropy is given by

$$\frac{S}{k_B} = -\sum_n P_n \ln P_n$$
$$= -\sum_n \frac{e^{-\beta E_n}}{Z(\beta)} [\ln e^{-\beta E_n} - \ln Z(\beta)]$$
$$= \beta U - \ln Z(\beta), \qquad (4.12)$$

where we used the expression of ensemble average energy to simplify to the last step.

4.3 Isoenergetic cycle

A new thermodynamic cycle composed of two isoentropic (adiabatic) and two isoenergetic processes is introduced in [4] and referred to as the *isoenergetic cycle* (Figure 4.2).

4.3.1 Isoentropic processes

In an isoentropic process, the occupation probabilities remain unchanged and the entropy remains constant.

Work done by a changing magnetic field is related to the magnetization $M = -\partial U/\partial B$, by dW = -MdB. If the magnetic field strength changes from B_{δ} to B_{γ} , the total work done is obtained as

$$W_{\delta \to \gamma} = \int_{B_{\delta}}^{B_{\gamma}} \frac{\partial U}{\partial B} dB = \int_{B_{\delta}}^{B_{\gamma}} \sum_{n} P_{n} \frac{dE_{n}(B)}{dB} dB$$
$$= \sum_{n} P_{n} [E_{n}(B_{\gamma}) - E_{n}(B_{\delta})]$$
(4.13)

The same result was derived in [6] for isoentropic processes directly, by identifying $dW = \sum_{n} P_n dE_n$ in the quantum version of the first law.

4.3.2 Isoenergetic processes

An isoenergetic process operates under the condition dU = 0, hence in a process $\delta \rightarrow \gamma$, the occupation probabilities and energy levels must change simultaneously to satisfy

$$\sum_{\mathbf{n}} E_{\mathbf{n}}(B_{\delta}) P_{\mathbf{n}}(B_{\delta}) = \sum_{\mathbf{n}} E_{\mathbf{n}}(B) P_{\mathbf{n}}(B) = \sum_{\mathbf{n}} E_{\mathbf{n}}(B_{\gamma}) P_{\mathbf{n}}(B_{\gamma}), \tag{4.14}$$

for every $B \in [B_{\delta}, B_{\gamma}]$. However, this relation is not sufficient to uniquely determine $P_{\mathbf{n}}(B)$ for every instant of the process. An exception to this is when the energy scale of the process is such that only transitions possible are between adjacent states.

External magnetic field is in the \hat{z} direction, therefore azimuthal symmetry of the system remains intact when the magnetic field is changed, and the *z*-component of angular momentum is conserved. As a result, the azimuthal quantum number doesn't change and we have the selection rule $\Delta m = 0$, for allowed transitions. If the system starts in the ground state (0,0), the only adjacent allowed state is (1,0). As a result, we have an effective two state system.

In the transition $1 \rightarrow 2$ as the magnetic flux density changes from B_{δ} to B_{γ} , we use (4.14) and the normalization condition $P_2(B) = 1 - P_1(B)$ to get for every $B \in [B_{\delta}, B_{\gamma}]$

$$E_{1}(B)P_{1}(B) + E_{2}(B)P_{2}(B) = E_{1}(B_{\delta})P_{1}(B_{\delta}) + E_{2}(B_{\delta})P_{2}(B_{\delta})$$
$$\implies P_{1}(B) = \frac{E_{2}(B_{\delta}) - E_{2}(B)}{E_{1}(B) - E_{2}(B)} + \frac{E_{1}(B_{\delta}) - E_{2}(B_{\delta})}{E_{1}(B) - E_{2}(B)}P_{1}(B_{\delta}).$$
(4.15)

Heat exchanged during the process is,

$$Q_{1\to2} = \int_{B_1}^{B_2} \left(P_1(B) \frac{dE_1}{dB} + P_2(B) \frac{dE_2}{dB} \right) dB$$

=
$$\int_{B_1}^{B_2} \left(P_1 \frac{d(E_1 - E_2)}{dB} + \frac{dE_2}{dB} \right) dB,$$
 (4.16)

which upon substituting (4.15) and an integration by parts, simplifies to

$$Q_{1\to2} = \{E_2(B_1) + [E_1(B_1) - E_2(B_1)]P_1(B_1)\}\ln\left[\frac{E_1(B_2) - E_2(B_2)}{E_1(B_1) - E_2(B_1)}\right].$$
(4.17)



Figure 4.2: Isoenergetic cycle in the effective two state system.

4.3.3 Isoenergetic cycle in the effective two state system

We consider a cycle that starts in the ground state with $P_1(B_1) = 1$.

1. Isoenergetic expansion $l_{B_1} \rightarrow l_{B_2}$ with $\alpha_1 = l_{B_2}/l_{B_1} > 0$. We assume that this process corresponds to maximal expansion, and the system ends up in the state (1,0): $P_1(B_2) = 0$ and $P_2(B_2) = 1$. Due to the conservation of energy $E_1(B_1) = E_2(B_2)$, we have

$$\begin{split} \hbar\omega_d \Bigg[1 + \frac{l_d^2}{2l_{B_1}^2} \Bigg]^{1/2} &= 3\hbar\omega_d \Bigg[1 + \frac{l_{B_1}^2}{l_{B_2}^2} \frac{l_d^2}{2l_{B_1}^2} \Bigg]^{1/2} \\ \implies 1 + \frac{l_d^2}{2l_{B_1}^2} &= 9 \Bigg[1 + \frac{l_d^2}{2\alpha_1^4 l_{B_1}^2} \Bigg] \\ \implies 1 + N_{\Phi_1}^2 &= 9 \Bigg[1 + \frac{N_{\Phi_1}^2}{\alpha_1^4} \Bigg], \end{split}$$
(4.18)

where we have identified $N_{\Phi_1} = \Phi_1/\Phi_0$ where $\Phi_0 = h/2e$ is the flux quantum, and $\Phi_1 = B_1(\pi l_d^2)$ is the magnetic flux through the quantum dot. Writing B_1 in terms of l_{B_1} and substituting gives $N_{\Phi_1} = l_d^2/2l_{B_1}^2$. We note that

$$\alpha_1 = \frac{(3N_{\Phi_1})^{1/2}}{(N_{\Phi_1}^2 - 8)^{1/4}},\tag{4.19}$$

has physically meaningful values when $N_{\Phi_1} > 8^{1/2}$; fixing a lower bound for the magnetic field B_1 . This constraint on the magnetic field is a result of requiring maximal expansion $(0,0) \rightarrow (1,0)$, in this step.

From (4.17), we get the expression for heat exchanged during the first stage

$$Q_{1\to2} = E_1(B_1) \ln\left[\frac{E_2(B_1) - E_1(B_1)}{E_2(\alpha_1^{-2}B_1) - E_1(\alpha_1^{-2}B_1)}\right],$$
(4.20)

and the work done $W_{1\rightarrow 2} = -Q_{1\rightarrow 2}$.

2. Isoentropic expansion $l_{B_2} \rightarrow l_{B_3}$, $\alpha = l_{B_3}/l_{B_2} > 1$. The expansion parameter α can be chosen arbitrarily. Work done in this process due to (4.13) is

$$W_{2\to3} = P_2(B_2)[E_2(B_3) - E_2(B_2)]$$

= $3\hbar\omega_d \left(\left[1 + \frac{N_{\Phi_1}^2}{(\alpha_1 \alpha)^4} \right]^{1/2} - \left[1 + \frac{N_{\Phi_1}^2}{\alpha_1^4} \right]^{1/2} \right).$ (4.21)

3. Isoenergetic compression The Landau radius is decreased $l_{B_3} \rightarrow l_{B_4}$ with $\alpha_3 = l_{B_4}/l_{B_3}$. Like the isoenergetic expansion, we assume that this process corresponds to maximal compression: $P_2(B_3) = P_1(B_4) = 1$. Maximal compression and the condition for energy conservation gives

$$\hbar\omega_{d} \left[1 + \frac{l_{d}^{2}}{2l_{B_{4}}^{2}} \right]^{1/2} = 3\hbar\omega_{d} \left[1 + \frac{l_{d}^{2}}{2l_{B_{3}}^{2}} \right]^{1/2}$$
$$\implies \hbar\omega_{d} \left[1 + \frac{N_{\Phi_{1}}^{2}}{(\alpha_{1}\alpha_{3}\alpha)^{4}} \right]^{1/2} = 3\hbar\omega_{d} \left[1 + \frac{N_{\Phi_{1}}^{2}}{(\alpha_{1}\alpha)^{4}} \right]^{1/2}, \qquad (4.22)$$

where we used the relations $l_{B_3} = \alpha l_{B_2} = \alpha(\alpha_1 l_{B_1})$, and $l_{B_4} = \alpha_3 l_{B_3} = \alpha_3(\alpha \alpha_1 l_{B_1})$. In particular, (4.22) fixes a value for the compression coefficient

$$\alpha_3 = \frac{N_{\Phi_1}^{1/2}}{[8(\alpha_1 \alpha)^4 + 9N_{\Phi_1}^2]^{1/4}}.$$
(4.23)

Again, the value of compression coefficient is fixed because we require maximal compression $(1,0) \rightarrow (0,0)$, in this step. Heat exchanged during this process is given by (4.17)

$$Q_{3\to4} = E_2(B_3) \ln\left[\frac{E_1(B_4) - E_2(B_4)}{E_1(B_3) - E_2(B_3)}\right],$$
(4.24)

where we use $l_B = [\hbar/m^*\omega_B]^{1/2} = [\hbar/eB]^{1/2}$ and the relations between l_{B_i} , i = 1, 2, 3, 4 in terms of the expansion/compression coefficients to get

$$B_3 = \frac{B_1}{(\alpha \alpha_1)^2}; \quad B_4 = \frac{B_1}{(\alpha \alpha_1 \alpha_3)^2}.$$
 (4.25)

The work performed is $W_{3\to4} = -Q_{3\to4}$.

4. Isoentropic compression This is the last step of the cycle which returns the system to the initial state. The Landau radius is reduced $l_{B_4} \rightarrow l_{B_1}$. The work done in this step is obtained from (4.13).

$$\begin{split} W_{4\to1} &= P_1[E_1(B_1) - E_1(B_4)] \\ &= \hbar \omega_d \Biggl(\left[1 + N_{\Phi_1}^2 \right]^{1/2} - \left[1 + \frac{N_{\Phi_1}^2}{(\alpha \alpha_1 \alpha_3)^4} \right]^{1/2} \Biggr) \\ &= 3\hbar \omega_d \Biggl(\left[1 + \frac{N_{\Phi_1}^2}{\alpha^4} \right]^{1/2} - \left[1 + \frac{N_{\Phi_1}^2}{(\alpha_1 \alpha)^4} \right]^{1/2} \Biggr) \\ &= -W_{2\to3}, \end{split}$$
(4.26)

where in the second step, we used the relations in (4.18) and (4.22), and in the third step we use (4.21). Hence the net work during the isoentropic process cancels $W_{2\rightarrow3} + W_{4\rightarrow1} = 0$.

4.3.4 Efficiency

We invoke (4.4) to write explicit expressions for $E_1(B)$ and $E_2(B)$:

$$E_{1}(B) = \hbar\Omega = \hbar\omega_{d} \left[1 + \frac{\omega_{B}^{2}}{4\omega_{d}^{4}} \right]^{1/2}$$
$$= \hbar\omega_{d} \left[1 + \left(\frac{l_{d}^{2}}{2l_{B}^{2}} \right)^{2} \right]^{1/2} = \hbar\omega_{d} \left[1 + N_{\Phi_{B}}^{2} \right]^{1/2}$$
(4.28)

and similarly,

$$E_2(B) = 3\hbar\omega_d \Big[1 + N_{\Phi_B}^2 \Big]^{1/2}.$$
(4.29)

We also note that

$$N_{\Phi_2} = \frac{N_{\Phi_1}}{\alpha_1^2}; \ N_{\Phi_3} = \frac{N_{\Phi_1}}{(\alpha \alpha_1)^2}; \ N_{\Phi_4} = \frac{N_{\Phi_1}}{(\alpha \alpha_1 \alpha_3)^2},$$
(4.30)

and define

$$\Theta(\alpha) = \left[1 + \frac{N_{\Phi_1}^2}{\alpha^4}\right]^{1/2},$$
(4.31)

in terms of which we write the energies are

$$E_1(B_1) = \hbar \omega_d \Theta(1); \qquad E_1(B_2) = \hbar \omega_d \Theta(\alpha_1); \tag{4.32}$$

$$E_1(B_3) = \hbar \omega_d \Theta(\alpha \alpha_1); \quad E_1(B_4) = \hbar \omega_d \Theta(\alpha \alpha_1 \alpha_3); \tag{4.33}$$

$$E_2(B_1) = 3\hbar\omega_d\Theta(1); \quad E_2(B_2) = 3\hbar\omega_d\Theta(\alpha_1);$$
 (4.34)

$$E_2(B_3) = 3\hbar\omega_d \Theta(\alpha \alpha_1); \ E_2(B_4) = 3\hbar\omega_d \Theta(\alpha \alpha_1 \alpha_3).$$
(4.35)

So that the expressions for heat exchange are

$$Q_{1\to2} = E_1(B_1) \ln \left[\frac{E_2(B_1) - E_1(B_1)}{E_2(B_2) - E_1(B_2)} \right]$$

= $\hbar \omega_d \Theta(1) \ln \left[\frac{\Theta(1)}{\Theta(\alpha_1)} \right]$ (4.36)

and

$$Q_{3\to4} = E_2(B_3) \ln\left[\frac{E_2(B_3) - E_1(B_3)}{E_2(B_4) - E_1(B_4)}\right]$$
$$= 3\hbar\omega_d \Theta(\alpha\alpha_1) \ln\left[\frac{\Theta(\alpha\alpha_1)}{\Theta(\alpha\alpha_1\alpha_3)}\right]$$
(4.37)

Efficiency of the cycle is given by the ratio

$$\eta(N_{\Phi_1}, \alpha) = 1 - \left| \frac{Q_{3 \to 4}}{Q_{1 \to 2}} \right|$$

= $1 - 3 \frac{\Theta(\alpha \alpha_1)}{\Theta(1)} \frac{\ln \left[\Theta(\alpha \alpha_1 \alpha_3) / \Theta(\alpha \alpha_1) \right]}{\ln \left[\Theta(1) / \Theta(\alpha_1) \right]}.$ (4.38)

When the field strength is very large $N_{\Phi_1} \gg 1$, the efficiency tends to the asymptotic limit

$$\eta \to 1 - \frac{1}{\alpha^2}.\tag{4.39}$$



Figure 4.3: Efficiency and work output for the isoenergetic cycle parametrised by magnetic flux.

4.4 Carnot cycle

The Carnot cycle consists of two isoentropic and two isothermal processes. During isothermal processes, the system is kept in equilibrium with a heat bath at a fixed temperature, and the occupation probabilities P_n satisfy the canonical distribution.

- 1. Isothermal expansion while in equilibrium with a heat bath at temperature $T_H = 1/k_B\beta_H$.
- 2. Isoentropic expansion in which no heat is exchanged with the environment.
- 3. Isothermal compression while in equilibrium with a heat sink at temperature $T_C = 1/k_B\beta_C$.
- 4. Isoentropic compression to reach the initial state.

4.4.1 Isothermal processes

During the isothermal process $\delta \rightarrow \gamma$ at temperature $T = 1/k_B\beta$, the heat exchanged is

$$Q_{\delta \to \gamma} = \int_{\delta}^{\gamma} \sum_{\mathbf{n}} E_{\mathbf{n}}(B) \frac{dP_{\mathbf{n}}(B)}{dB} dB$$

= $\left[\sum_{\mathbf{n}} P_{\mathbf{n}}(B)E_{\mathbf{n}}(B)\right]_{B_{\delta}}^{B_{\gamma}} - \int_{\delta}^{\gamma} \sum_{\mathbf{n}} \frac{dE_{\mathbf{n}}}{dB} P_{\mathbf{n}}(B) dB$
= $\left[U(B_{\gamma}) - U(B_{\delta})\right] + \int_{\delta}^{\gamma} \frac{1}{\beta} \frac{d\ln Z(B,\beta)}{dB} dB$
= $\left[U(B_{\gamma}) - U(B_{\delta})\right] + \frac{1}{\beta} \ln \left[\frac{Z(B_{\gamma},\beta)}{Z(B_{\delta},\beta)}\right],$ (4.40)

where we used the following fact

$$\frac{\mathrm{d}\ln Z(B,\beta)}{\mathrm{d}B} = \frac{1}{Z(B,\beta)} \frac{\mathrm{d}}{\mathrm{d}B} \sum_{\mathbf{n}} e^{-\beta E_{\mathbf{n}}}$$
$$= \sum_{\mathbf{n}} -\beta \frac{e^{-\beta E_{\mathbf{n}}}}{Z(B,\beta)} \frac{\mathrm{d}E_{\mathbf{n}}}{\mathrm{d}B} = -\beta \sum_{\mathbf{n}} P_{\mathbf{n}}(B) \frac{\mathrm{d}E_{\mathbf{n}}}{\mathrm{d}B}.$$
(4.41)

Hence we have the following expressions of heat absorbed and rejected during the isothermal processes

$$Q_{1\to 2} = U(B_2) - U(B_1) + \frac{1}{\beta_H} \ln\left[\frac{Z(B_2, \beta_H)}{Z(B_1, \beta_H)}\right],$$
(4.42)

$$Q_{3\to4} = U(B_4) - U(B_3) + \frac{1}{\beta_C} \ln\left[\frac{Z(B_4, \beta_C)}{Z(B_3, \beta_C)}\right].$$
(4.43)

4.4.2 Isoentropic processes

The isoentropic condition $\Delta S = 0$, imposes bounds on the strength of the magnetic field and we have

$$\Delta S_{2\to3} = 0 = S(B_3, \beta_C) - S(B_2, \beta_H)$$

= [\beta_C U(\beta_C, B_3) + \ln Z(B_3, \beta_C)] - [\beta_H U(\beta_H, B_2) + \ln Z(B_2, \beta_H)] (4.44)

$$\Delta S_{4\to 1} = 0 = S(B_1, \beta_H) - S(B_4, \beta_C)$$

= [\beta_H U(\beta_H, B_1) + \ln Z(B_1, \beta_H)] - [\beta_C U(\beta_C, B_4) + \ln Z(B_4, \beta_C)] (4.45)

Combining the two expressions in (4.44) and (4.45) leads to

$$\beta_{C}[U(B_{3},\beta_{C}) - U(B_{4},\beta_{C})] + \ln\left[\frac{Z(B_{3},\beta_{C})}{Z(B_{4},\beta_{C})}\right]$$

$$= \beta_{H}[U(B_{2},\beta_{H}) - U(B_{1},\beta_{H})] + \ln\left[\frac{Z(B_{2},\beta_{H})}{Z(B_{1},\beta_{H})}\right]$$

$$\Longrightarrow -\frac{Q_{3\rightarrow 4}}{\beta_{H}} = \frac{Q_{1\rightarrow 2}}{\beta_{C}}$$

$$\Longrightarrow \quad \frac{Q_{3\rightarrow 4}}{Q_{1\rightarrow 2}} = -\frac{\beta_{H}}{\beta_{C}}, \quad (4.46)$$

where we used (4.42) and (4.43) to identify the quantities in the above equations as the heat absorbed and rejected during isothermal cycles.

4.4.3 Work and efficiency

Work output in the Carnot cycle is simply,

$$W = Q_{1 \to 2} - Q_{3 \to 4}$$

= $\left(1 - \frac{Q_{3 \to 4}}{Q_{1 \to 2}}\right)Q_{1 \to 2}$
= $\left(1 - \frac{T_C}{T_H}\right)\left(U(B_2) - U(B_1) + \frac{1}{\beta_H}\ln\left[\frac{Z(B_2, \beta_H)}{Z(B_1, \beta_H)}\right]\right),$ (4.47)

where in the second step we used (4.46), which we also use to write the efficiency of the Carnot cycle as

$$\eta = 1 - \left| \frac{Q_{3 \to 4}}{Q_{1 \to 2}} \right| = 1 - \frac{T_C}{T_H},\tag{4.48}$$

which is identical to the efficiency of the classical Carnot cycle, and consistent with what was derived in the previous chapter with more general considerations.

5 Conclusion

A very large part of this project was dedicated to studying thermodynamic cycles in the quantum world, and comparing their properties to their classical counterparts. We started with a quantum description of the Szilard engine, which despite having work output identical to the classical cycle, showed some very dramatic departures from classical behaviour. In particular, the non-zero work required in the insertion of the barrier, and the starkly different work outputs for bosons and fermions were noted to be manifestly quantum effects.

In the following chapter, the quantum analogues of several thermodynamic processes were described, and the quantum versions of common classical heat engine cycles built. Derivation of operational efficiencies and work output were done with extremely general considerations in the spirit of classical thermodynamics; the quantum nature of the working substances was abstracted away and assumed to be contained in the partition function. Hence, it is not surprising that the efficiencies of quantum heat engine cycles were identical to their classical counterparts. In particular, it was observed that the efficiency and the positive work condition of the quantum Carnot cycle depends on only the temperatures of the reservoirs between which the engine operates, and not on any details of the working substance.

The penultimate chapter describes a physically realizable quantum heat engine in the context of a quantum dot. An isoenergetic cycle was described for an effective two level system and exact analytic expressions were derived for how the magnetic flux density must be changed in each step of the cycle. In the Carnot cycle based on the quantum dot, the classical efficiency was recovered, pointing to the consistency of the framework presented in [6].

5.1 Future work

In this report, the thermodynamic cycles were studied in the context of two physical systems: single-mode radiation field in a cavity, and a magnetically controlled particle in a cylindrical potential well. For future work, I intend to study alternative thermodynamic cycles based on different quantum systems. In particular, I will study the magnetostrain driven quantum heat engine based on a graphene flake as presented in [9].

A Classical Thermodynamic Cycles

This appendix presents a summary of the classical versions of the Otto and Carnot cycles.

A.1 Otto cycle

The classical Otto cycle consists of six strokes (Figure A.1).



Figure A.1: Classical Otto cycle.

- $0 \rightarrow 1$ *Intake stroke*. We model this process by a quasistatic isobaric process. The volume of the chamber goes from zero to V_1 and the working substance is is pushed into the engine according to the equation of state $P_0V = nRT_1$, where P_0 is the atmospheric pressure, *n* is the number of moles of working substance, and T_1 is the ambient temperature.
- $1 \rightarrow 2$ *Compression stroke* is modelled by a quasistatic adiabatic compression process. The temperature rises from T_1 to T_2 according to equation

$$T_1 V_1^{\gamma - 1} = T_2 V_2^{\gamma - 1}, \tag{A.1}$$

where $\gamma = C_P / C_V$.

- $2 \rightarrow 3$ *Combustion* During combustion, the piston remains almost stationary, and the temperature increases further. We model this by a quasistatic isochoric process, in which the temperature increase is brought about absorption of heat Q_H from a series of external high temperature reservoirs whose temperatures range from T_2 to T_3 .
- $3 \rightarrow 4$ *Power stroke* is approximated by an adiabatic expansion that leads to a drop in temperature from T_3 to T_4 , according to the equation

$$T_3 V_2^{\gamma - 1} = T_4 V_1^{\gamma - 1}, \tag{A.2}$$

 $4 \rightarrow 1$ *Exhaust* is an quasistatic isochoric drop in temperature and pressure of *n* moles of gas brought about by a series of heat reservoirs whose temperatures range from T_4 to T_1 , where T_1 is the ambient temperature.

 $1 \rightarrow 0$ *Exhaust stroke* Represents an isobaric process at atmospheric pressure in which the gas is ejected from the chamber, and its volume goes from V_1 to zero.

A.1.1 Efficiency

The isobaric processes $0 \rightarrow 1$ and $1 \rightarrow 0$ cancel each other and need not be considered. The work done in the cycle is the difference between Q_H the heat absorbed at high temperatures from $2 \rightarrow 3$, and Q_L the heat rejected at lower temperatures from $4 \rightarrow 1$.

Heat absorbed in the isochoric process $2 \rightarrow 3$ is given

$$|Q_{2\to3}| = \int_{2}^{3} C_V dT = C_V (T_3 - T_2), \qquad (A.3)$$

and the heat rejected in the process $4 \rightarrow 1$ is

$$|Q_{4\to 1}| = \int_{4}^{1} C_V dT = C_V (T_4 - T_1).$$
 (A.4)

This leads to the following expression for thermal efficiency

$$\eta_0 = 1 - \left| \frac{Q_{4 \to 1}}{Q_{2 \to 3}} \right| = 1 - \frac{T_4 - T_1}{T_3 - T_2}.$$
(A.5)

From (A.1) and (A.2) we get $T_1/T_4 = T_2/T_3$ which can be used to obtain,

$$\frac{T_4 - T_1}{T_3 - T_2} = \frac{T_1}{T_2},\tag{A.6}$$

which we use to simplify the expression of efficiency

$$\eta_0 = 1 - \frac{T_1}{T_2}.$$
 (A.7)

A.2 Carnot cycle



Figure A.2: Classical Carnot cycle.

We shall look at a Carnot cycle with an ideal gas as working substance. Initially, the gas is in a state represented by the point 1 (Figure A.2). The four processes of the cycle are

- 1. Process $1 \rightarrow 2$ is reversible adiabatic compression until the temperature rises to T_H .
- 2. Process $2 \rightarrow 3$ is reversible isothermal expansion at temperature T_H .
- 3. Process $3 \rightarrow 4$ is reversible adiabatic expansion until the temperature drops to T_c .
- 4. Process $4 \rightarrow 1$ is reversible isothermal compression at T_C until the initial state is reached.

A.2.1 Efficiency

Heat Q_H , is absorbed during the cycle in the isothermal process $2 \rightarrow 3$, which is calculated as

$$Q_{2\to3} = \int_{2}^{3} T \,\mathrm{d}S = T_H(S_3 - S_2),\tag{A.8}$$

and heat Q_C is rejected during the isothermal process $4 \rightarrow 1$

$$Q_{4\to 1} = \int_{1}^{4} T \,\mathrm{d}S = T_C(S_4 - S_1). \tag{A.9}$$

In the adiabatic processes no heat is exchanged, therefore dS = dQ/T = 0. This gives us $S_1 = S_2$ and $S_3 = S_4$. This relation between entropies is used to simplify thermal efficiency

$$\eta_C = 1 - \left| \frac{Q_{4 \to 1}}{Q_{2 \to 3}} \right| = 1 - \frac{T_C}{T_H}.$$
(A.10)

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