OPTIMIZED EFFICIENCY OF A MODEL QUANTUM HEAT ENGINE WORKING IN A FINITE TIME

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Abstract

In this work we consider spin-half particle with two energy levels in contact with two heat reservoirs and we apply magnetic field on it whose task is to convert the input energy from the hot reservoir and from the magnetic field to useful work. We analytically study the optimized quantum thermodynamic efficiency, which lies between Carnot efficiency and efficiency at maximum power. We also find the time taken to accomplish one complete cycle at the maximum power and at optimized efficiencies.

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Chapter 1

Introduction

Thermodynamics is the study of the connection between heat and work and the conversion of one into the other. This study is important because many machines and modern devices change heat into work (such as an automobile engine) or turn work into heat(or cooling as in a refrigerator).

In the development of the second law of thermodynamics, it is very useful to define a hypothetical body with a relatively large thermal energy capacity that can supply or absorb finite amounts of heat without undergoing any change in temperature. Such a body is called reservoir. A reservoir that supplies energy in the form of heat is considered as a source, and one that absorbs energy in the form of heat is considered as a sink. In practice, large bodies of water such as oceans, lakes and rivers as well as the atmospheric air can be modeled accurately as a heat reservoir because of their large thermal energy storage capacities or thermal masses.

Work can be converted to heat directly and completely, but converting heat to work requires the use of some special devices. We call such devices as heat engines. A heat engine is a device which converts the heat energy into work. Heat engines are characterized by three attributes: the working medium, the cycle of operation, and the dynamics that govern the cycle.

Figure 1.1 schematically represents a heat engine as shown below.

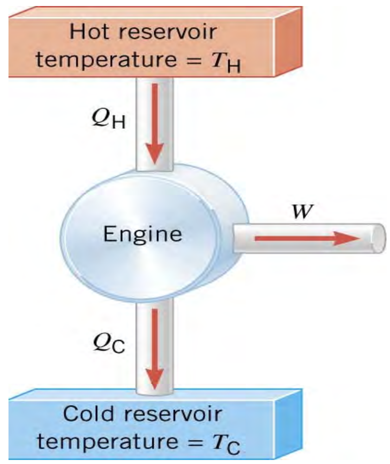


Figure 1.1: Schematic representation of a heat engine

As we see from the above diagram, the engine absorbs a quantity of energy Q_h from the hot reservoir, does work W, and then gives up a quantity of energy Q_c to the cold reservoir. Heat engines differ considerably from one another, but all can be characterized by the following.

1. They receive heat from a high-temperature source (solar energy, oil furnace, nuclear reactor, etc.).

2. They convert part of this heat to work (usually in the form of a rotating shaft).

3. They reject the remaining waste heat to a low-temperature sink (the atmosphere, rivers, etc.).

4. They operate on a cycle

Heat engines and other cyclic devices usually involve a fluid to and from which heat is transferred while undergoing a cycle. This fluid is called the working fluid.

Cyclic heat engines utilize a working gas that moves through a reversible cycle to transfer heat between hot and cold heat reservoirs and do useful work [1]. A working gas may be defined as a system that is at all times close to thermal equilibrium, so that it has well-defined state variables such as temperature.

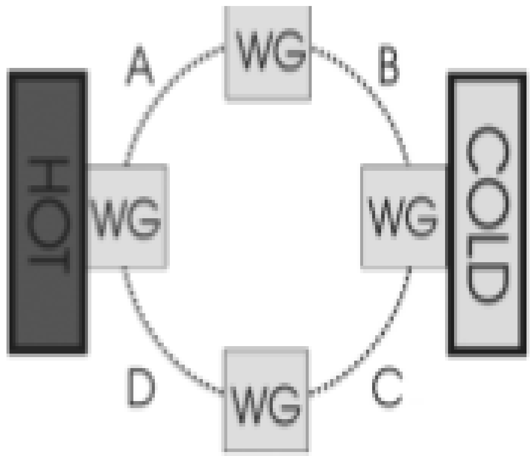


Figure 1.2: Schematic of a cyclic heat engine[1]. The essential components are two heat reservoirs and a working gas (WG) that is cycled through a series of quasi-equilibrium states with well-defined temperature.

In general, the efficiency of a given heat transfer process (whether it be a refrigerator, a heat pump or an engine) is defined informally by the ratio of "what you get out" to "what you put in". Therefore, the efficiency of the heat engine is defined as the ratio of the net work done per cycle by the engine to the amount of the heat absorbed per cycle by the working substance from the source and it is denoted by η, so that

$$\eta = \frac{W}{Q_h} = \frac{Q_h - Q_c}{Q_h} = 1 - \frac{Q_c}{Q_h}. \tag{1.1}$$

The theoretical maximum efficiency of any heat engine depends only on the temperatures within which it operates. This efficiency is usually derived using an ideal imaginary heat engine such as the Carnot heat engine. Empirically, no engine has ever been shown to run at a greater efficiency than that of Carnot cycle heat engine because they do not operate through a reversible cycle. Thus, the efficiency η_c of a Carnot heat engine is.

$$\eta_c = 1 - \frac{T_c}{T_h}. \tag{1.2}$$

where T_h and T_c are the temperatures of the hot and cold reservoirs, respectively. The practical implications of Carnot efficiency is limited since the upper limit η_c ("Carnot efficiency") is only reached for engines that operate reversibly. To operate reversibly, the process must be done quasi-statically which requires infinite amount of time for each cycle. As a result, when the efficiency is maximal, the output power is zero. By optimizing the Carnot cycle with respect to power rather than efficiency, Curzon and Ahlborn [2] introduced a Carnot-like thermal engine in which there is no thermal equilibrium between the working fluid and the thermal reservoirs at the isothermal branches of the cycle. These authors demonstrated that such an engine produces nonzero power (contrary to the Carnot engine), and that the power output can be optimized by varying the temperature of the cycle's isothermal branches. The efficiency under these conditions is

$$\eta_{CA} = 1 - \sqrt{\frac{T_c}{T_h}}. \tag{1.3}$$

Hernandez et.al [3] have come up with a unified optimization criterion (Ω criterion) to identify the point of operation of an engine where trade-off between energy cost and fast transport is compromised. By applying this optimization criterion we can get the efficiency in between Carnot and maximum power efficiency. In addition to comparing the optimized efficiency with Carnot efficiency and maximum power efficiency we also calculate optimized power and optimized time to complete the full cycle.

In this work we take a spin-half particle with two energy levels as heat engine in contact with two heat reservoirs at different temperatures and there is a magnetic field which we apply on it.

The rest of the thesis is organized as follows. In Chapter two we demonstrate a model which is considered by H.T. Quan, Yu-xi Liu, C. P. Sun, and Franco Nori of Quantum thermodynamic cycles and quantum heat engines. In Chapter three we develop a model which is spin-half particle with two energy levels as a working substance inside the magnetic field and connected with two heat reservoirs at different temperatures, and by maximizing output power in-terms of time we calculate maximum power efficiency and the minimum time required to perform one cycle. In Chapter four we develop an objective function based on the proposal of Hernandez et.al.[3] and using optimization principle we optimize the objective function with respect to time, t, and then we calculate the optimized efficiencies of the model and the optimized times taken to perform one cycle. We put summary and conclusion of the whole work in the last Chapter.

Chapter 2

Quantum Thermodynamic Cycles and Quantum Heat Engines

In this chapter we are going to demonstrate a quantum isothermal process with infinite number of infinitesimal quantum adiabatic process (QAP) and quantum isochoric process (QIP), which is presented by H.T. Quan, Yu-xi Liu, C. P. Sun, and Franco Nori.

2.1 Basic Quantum Thermodynamic Process

2.1.1 Quantum first law of thermodynamics

To define quantum isothermal and quantum isochoric processes, we need to first consider the working substance. An arbitrary non-interacting quantum system with a finite number of energy levels is used. The Hamiltonian of the working substance can be written as

$$H = \sum_n E_n |n\rangle\langle n|. \tag{2.1}$$

Where $|n\rangle$ is the n^{th} eigen-state state of the system and E_n is its corresponding eigen-energy. The internal energy U of the working substance can be expressed as

$$U = \sum_n E_n p_n, \tag{2.2}$$

for a given occupation distribution with probabilities p_n in the n^{th} eigen-state. To clearly define quantum isothermal and isochoric processes, we need to identify the quantum analogues of the infinitesimal heat exchange dQ and the infinitesimal work performed dW. From Eq.(2.2) we have

$$dU = \sum_n [E_n dp_n + p_n dE_n]. \tag{2.3}$$

In classical thermodynamics, the first law of thermodynamics is expressed as

$$dU = dQ + dW, \tag{2.4}$$

where $dQ = TdS$ (T is the temperature and S is the entropy), $dW = \sum_i Y_i dy_i$[4, 5] (y_i is the generalized coordinate and Y_i is the generalized force conjugated to y_i). Due to the relationship $S = k_B \sum_i p_i ln p_i$ between the entropy S and the probabilities p_i, we can make the following identification

$$dQ = \sum_n E_n dp_n, \tag{2.5}$$

and

$$dW = \sum_n p_n dE_n. \tag{2.6}$$

Equation (2.6) implies that the work performed corresponds to the change in the eigen energies E_n, and this is in accordance with the fact that work can only be performed through a change in the generalized coordinates of the system, which in turn gives rise to a change in the eigen energies[6]. Thus the quantum version of the first law of thermodynamics $dU = dQ + dW$ just follows from Eq.(2.3) with the quantum identifications of heat exchange and work performed in Eqs.(2.5) and (2.6). Different from dQ = T dS, which is applicable only to the thermal equilibrium case, below we will see that Eqs. (2.5) and (2.6) are applicable to both the thermal equilibrium case.

2.1.2 Quantum isothermal process

Consider the quantum versions of some thermodynamic processes[7]. In quantum isothermal processes, the working substance, such as a particle confined in a potential energy well, is kept in contact with a heat bath at a constant temperature[7]. The particle can perform positive work to the outside, and meanwhile absorb heat from the bath. Specifically, in this work consider a two level system with the excited state $|e\rangle$, the ground state $|g\rangle$, and a single energy spacing Δ with instantaneous eigen energy $(E_e(t)$ $(E_g(t))$ depending on time t. We modeled this two-level system as a spin-1/2 particle in an external magnetic field. It interacts with a heat bath of inverse temperature β, which can be universally modeled as a collection of many bosons. Initially, the two-level system is in thermal equilibrium. Then by altering the magnetic field slowly the energy level spacing $\Delta(t)$ slowly changes from Δ_A to Δ_B. During the controlling process (by changing magnetic field at constant temperature) illustrated by the smooth curve $\widetilde{AB}$ in Fig.(2.1), work is done on the system. In the infinitely slow process, which can be alternatively regarded as a quantum isothermal process the two-level system is in the thermal equilibrium at every instant.

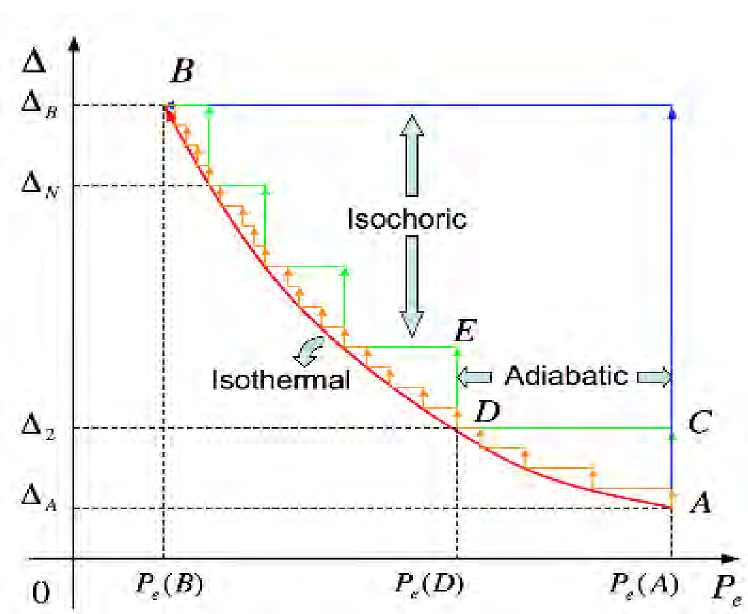


Figure 2.1: Schematic illustration of a quantum isothermal process[8]$\widetilde{AB}$. Here the horizontal axis P_e is the occupation probability in the excited state of the two-level system, and the vertical axis indicates the level spacing of the two-level system. The smooth curve $\widetilde{AB}$ represents the isothermal process, whose equation of state can be expressed as $\Delta(t) = -\beta^{-1} ln(p_e^{-1} - 1)$. The horizontal and vertical lines represent QIP and QAP[8].

It should be pointed out that, during the isothermal process, there is a heat exchange between the two-level system and the heat bath. For such an isothermal process, it is difficult to calculate the microscopic work distribution directly. According to Ref.[8], however, this process can be simulated by a series of QAP and QIP. In QAP (QIP) processes, there is only work done (heat exchange). Hence, using the changes of eigen-energies of microscopic state at instant t = A, C, D, it is possible to calculate the microscopic work done (heat exchange) $dW = E_\alpha(C) - E_\alpha(A)$ $[dQ = E_\alpha(D) - E_\beta(C)]$ for α ,$\beta = e, g$ [9]. In the parameter space, these QAP and QIP series processes are represented by the stair path $(A \to C \to D \to \cdots \to B)$ in Fig.2.1 . When every step of the stair path becomes infinitesimal, the stair path becomes equivalent to the isothermal process $\widetilde{AB}$. In this way they simulate the quantum isothermal process with N equal-height steps with the small height $\Delta = \frac{(\Delta_B - \Delta_A)}{N}$ where Δ_A and Δ_B are the level spacings at point A and point B, respectively. The level spacings of the two-level system after the $(j-1)^{th}$ QIP is

$$\Delta_j = \Delta_A + (j-1)\Delta. \tag{2.7}$$

for $j = 1, 2, \cdots, N+1$. The initial and final point A, and B, corresponds to $j = 1$ and $j = N+1$, respectively. Put the initial point A, and the final point B, the jump Δ in every step decrease with increase of the step number N , and Δ approaches zero when N becomes infinity. Obviously, when $N \to \infty$, the stair path approaches its asymptotic behavior the isothermal path (see Fig. 2.1). When the system reaches thermal equilibrium, the occupation probabilities obeys the Gibbs distribution defined by

$$p_e^j = \frac{e^{-\beta\Delta_j}}{1 + e^{-\beta\Delta_j}}; p_g^j = p_e^j e^{\beta\Delta_j}. \tag{2.8}$$

Having defined the path in the parameter space (Δ, P_e), and further introduce the microscopic work and its corresponding probabilities for a given path. In the above path divided into many steps, the first step $A \to C \to D$ consists of a QAP $A \to C$, and a QIP $C \to D$. At the beginning (the point A of Fig. 2.1), the system is initially in a thermal equilibrium state, which implies that the system is either in its microscopic state $|g\rangle$ or $|e\rangle$ with probabilities p_g or p_e respectively. We choose the ground state in the energy reference point so that the microscopic energy $E(A)$ of the system at initial point A can take $E_e(A) = \Delta_A$ or $E_g(A) = 0$, with probability p_e and $1 - p_e$ respectively. In the first QAP $A \to C$, the system remains in its microscopic state $|g\rangle(|e\rangle)$ if the system is initially in its microscopic state $|g\rangle(|e\rangle)$. As there is no heat exchange in the quantum adiabatic process, the work done by external parameter (such as magnetic field) is just the change of the microscopic energy $W = E_\alpha(C) - E_\alpha(A)$ for $\alpha = e, g$. Correspondingly, the work done during $A \to C$ can be either $\Delta_C - \Delta_A$ or 0 with probabilities p_e or $1 - p_e$ respectively. This also agrees with the definition of work in quantum mechanical system: work is associated with the change of the level spacing.

2.1.3 Quantum isochoric process

A quantum isochoric process has similar properties to that of a classical isochoric processes. In a quantum isochoric process, the working substance is placed in contact with a heat bath. No work is done in this process while heat is exchanged between the working substance and the heat bath[4]. This is the same as that in a classical isothermal process. In a quantum isochoric process the occupation probabilities p_n and thus the entropy S change, until the working substance finally reaches thermal equilibrium with the heat bath. In classical isochoric process the pressure P and the temperature T change, and the working substance reaches thermal equilibrium with the heat bath only at the end of this process. For example, if the working substance is chosen to be a particle confined in a infinite square well potential, no work is done during a quantum isochoric process when heat is absorbed or released, and the occupation probabilities in every eigen state satisfy Boltzmann distribution at the end of the isochoric process.

2.1.4 Quantum adiabatic process

A classical adiabatic thermodynamic process can be formulated in terms of a microscopic quantum adiabatic thermodynamic process. Because quantum adiabatic processes proceed slow enough such that the generic quantum adiabatic condition is satisfied, then the population distributions remain unchanged, $dp_n = 0$.

According to Eq(2.5), dQ = 0, there is no heat exchange in a quantum adiabatic process, but work can still be nonzero according to Eq(2.6). A classical adiabatic process, however, does not necessarily require the occupation probabilities to be kept invariant.

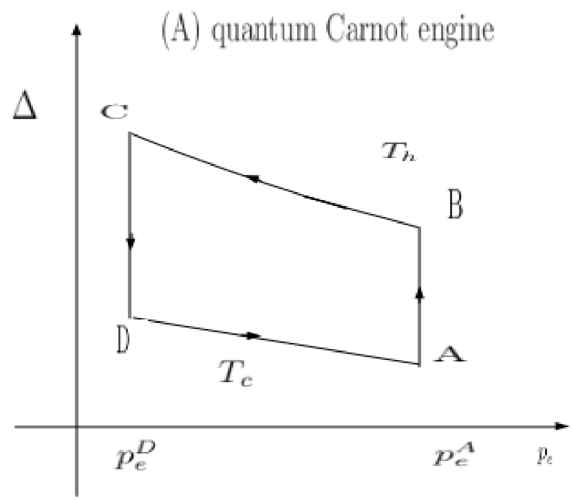
We can see the difference and similarity between quantum and classical thermodynamic processes in the table below.

	Isothermal process	Isochoric process	Adiabatic process
Classical	Heat absorbed or released. Work done. INV: U, T VAR: P, V	Heat absorbed or released. No work done. INV: V VAR: P, T	No heat exchange. Work done. VAR: P, T, V
Quantum	Heat absorbed or released. Work done. INV: T VAR: U, E_n, p_n	Heat absorbed or released. No work done. INV: E_n VAR: p_n, T_{eff}	No heat exchange. Work done. INV: p_n VAR: E_n, T_{eff}

Table 2.1: Quantum versus classical thermodynamic processes[7]. Here we use INV to indicate the invariance of a thermodynamic quantity and VAR to indicate that it varies or changes. U is the internal energy of the working substance; T temperature of the reservoir, $T_{eff}=\frac{\Delta}{k_B}[\ln(\frac{p_g}{p_e})]^{-1}$, P pressure of ideal gas, E_n is the n-th eigen state energy of the working substance, p_n is the n-th eigen state probability of the working substance and v is volume of the ideal gas. The working substance of the classical thermodynamic processes considered here is the ideal classical gas.

2.2 Quantum Carnot Engine Cycle(QCE)

In the previous section, we defined quantum isothermal and adiabatic processes. Based on this definition, in this section, we study the QCE cycle and its properties. The QCE cycle (see Fig.2.2 for our model of a QCE based on a two-level spin-half particle system inside a magnetic field), which is different from H.T. Quan, Yu-xi Liu, C. P. Sun, and Franco Nori model (the two-level particle system confined in the potential well). Like its classical counterpart, consists of two quantum adiabatic processes (A $\rightarrow$ B and C $\rightarrow$ D) and two quantum isothermal processes (B $\rightarrow$ C and D $\rightarrow$ A). During the isothermal expansion process from B to C, the spin-half particle inside the magnetic field which is kept in contact with a heat bath at temperature T_h , while the energy levels of the system change much slower than the relaxation of the system, so that the particle is always kept in thermal equilibrium with the heat bath.



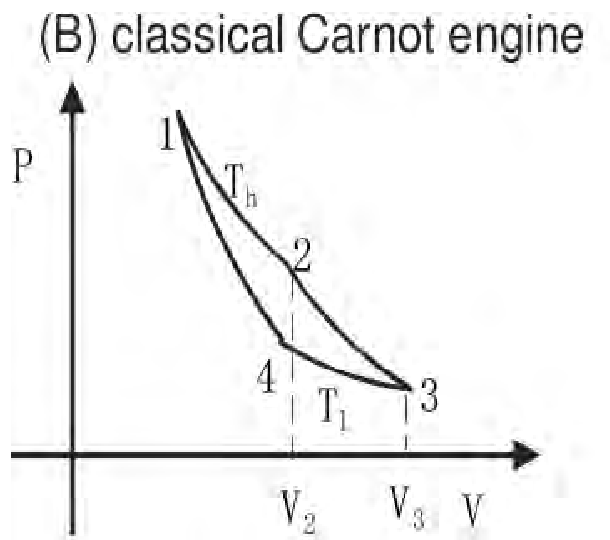


Figure 2.2: (A): A schematic diagram of a quantum Carnot engine based on a two-level quantum system. Δ is the level spacing between the two energy levels. p_e is the occupation probability in the excited state. The process from B to C (D to A) is the isothermal expansion (compression) process, in which the spin-half particle is inside a magnetic field and put in contact with the high (low) temperature heat bath. The processes from A to B and from C to D are two adiabatic processes. (B): Pressure-Volume (P V) diagram for a classical Carnot engine with ideal gas as the working substance. The process from 1 to 2 (from 3 to 4) is the classical isothermal expansion (compression) process with temperature T_h (T_l), and the process from 2 to 3 (4 to 1) is the classical adiabatic expansion (compression) process. V_2 and V_3 are the volume of the working substance at 2 and 3 respectively.

Now we will see how it is possible to analyze the operation efficiency η_C of the QCE. For simplicity use $dQ = TdS$ to calculate the heat exchange dQ in any Quantum Iso Thermal (QIT) process. Because the temperature of the heat bath is kept invariant in the quantum isothermal process, the heat absorbed Q_{in} and released Q_{out} in the quantum isothermal expansion and compression processes can be calculated as follows.

$$Q_{in} = T_h[S(C) - S(B)] \tag{2.9}$$

$$Q_{out} = T_c[S(A) - S(D)] \tag{2.10}$$

where T_h and T_c are the temperatures of the two different heat reservoirs.

$$S(i) = -k_B \sum_n p_i ln p_i \tag{2.11}$$

are the entropies of the working substance at different instants $i = A\ ,B,\ C\ ,D$, and calculating the work W_{cyc} done during a QCE cycle and its operation efficiency η_c. From Eqs.(2.9) and (2.10) and the first law of thermodynamics we obtain the net work done during a QCE cycle is

$$W_{cyc} = Q_{in} + Q_{out}. \tag{2.12}$$

$$W_{cyc} = (T_h - T_c)[S(C) - S(B)], \tag{2.13}$$

where we have used the relations $S(B) = S(A)$ and $S(C) = S(D)$. This equivalence is due to the fact that the occupation probabilities and thus the entropy remain invariant in any quantum adiabatic process. The efficiency η_c of the QCE is

$$\eta_c = \frac{W_{cyc}}{Q_{in}}, \tag{2.14}$$

which is just the efficiency of a classical Carnot engine

$$\eta_c = 1 - \frac{T_c}{T_h}. \tag{2.15}$$

Internal energy

It is well known that an ideal classical Carnot engine cycle consists of two classical isothermal and two classical adiabatic processes. When the working substance is the ideal gas, the internal energy of the working substance remains invariant in the classical isothermal process, because the internal energy of the ideal gas depends on the temperature only. This assumption for classical isothermal processes based on classical ideal gas could be true for a classical Carnot engine using a working substance other than an ideal gas. But in the quantum version, the quantum isothermal and quantum adiabatic processes should be redefined microscopically based on quantum mechanics. In principle, the classical result could change when considering the quantum nature (discrete energy levels) of the working substance.

Now by using this concept as a base in the next two chapters we are going to introduce the model of finite time quantum Carnot engine and drive quantities such as maximum power efficiency, optimized efficiencies, optimized powers and optimized time to complete one cycle.

Chapter 3

Efficiency at maximum power for a two level quantum system

3.1 model of the system

We consider a two-level quantum mechanical system with excited (ground) states $|e>$ ($|g>$) with instantaneous eigen-energy E_e (E_g). This two-level system can be modeled as a spin-1/2 in an external magnetic field. It interacts with a heat bath of inverse temperature β, which can be universally modeled as a collection of many bosons. Consider a one cycle process, it is difficult for such a cyclic process containing an isothermal process to calculate the microscopic work and heat transfer directly. So, we can divide the isothermal expansion and compression into a series of N steps of quantum adiabatic processes (QAP) and quantum isochoric processes (QIP) in which the magnetic field is changed slowly.

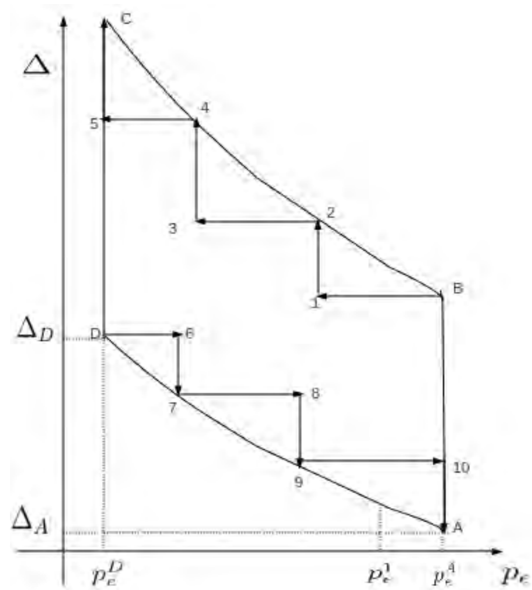


Figure 3.1: Schematic illustration of a quantum Carnot cycle for finite time division (N=3).

Assuming from the above diagram the system is equilibrium at point A initially and also gets equilibrium after consecutive isochoric expansion (compression). Using extended concept of the quasi static limit we can determine the heat and work in every step. The basic problem that we address is the finite-time performance of this engine as it runs through the following four standard stages of a Carnot cycle also see the above figure.

3.1.1 Adiabatic process

The spin-half particle is disconnected from the cold reservoir, and the quantum level is shifted from A to B. Since the spin-half particle is thermodynamically isolated, the population of the level does not change during this process. Hence, there is no heat exchange. However, the change of the energy level absorbs a corresponding amount of work. We assume that the operation time of this step is very short, in particular negligibly small compared to that of the isothermal processes.

3.1.2 Isothermal process

The spin-half particle is connected to the hot temperature T_h. The energy level is increased from B to C based on another protocol during a time interval of length n. Both heat and work are exchanged. Now the total heat absorbed in this process is simply the sum of the three individual absorbed heat energies.

i.e,

$Q_{In} = \Delta Q^1 + \Delta Q^2 + \Delta Q^3$.

In the first step it will absorb

$$\Delta Q^1 = (E_e^1 - E_g^1)(p_e^1 - p_e^B), \tag{3.1}$$

in the second step it will absorb

$$\Delta Q^2 = (E_e^2 - E_g^2)(p_e^3 - p_e^2), \tag{3.2}$$

and in the third step it will absorb

$$\Delta Q^3 = (E_e^3 - E_g^3)(p_e^5 - p_e^4). \tag{3.3}$$

There for the total heat absorbed will be

$$Q_{In} = \Delta Q^1 + \Delta Q^2 + \Delta Q^3. \tag{3.4}$$

By inserting the value calculated above we can get the absorbed heat energy as follow.

$$Q_{In} = (E_e^1 - E_g^1)(p_e^1 - p_e^B) + (E_e^2 - E_g^2)(p_e^3 - p_e^2) + (E_e^3 - E_g^3)(p_e^5 - p_e^4). \tag{3.5}$$

Taking the occupation probabilities $p_e^B = p_e^A$, $p_e^1 = p_e^2$, $p_e^3 = p_e^4$, $p_e^5 = p_e^C$, and after taking this in Eq.(3.5) we get Q_{In} in the following form.

$$Q_{In} = (E_e^C - E_g^C)p_e^C - (E_e^B - E_g^B)p_e^B - \Delta(p_e^C + p_e^2 + p_e^4). \tag{3.6}$$

3.1.3 Adiabatic process

The system is again disconnected from the hot reservoir and the level is restored from C to D, at the cost of a corresponding amount of work. Afterwards, the spin-half particle is reconnected to the cold lead. Again, we assume that the operation time of this process is negligibly small.

3.1.4 Isothermal process

The spin-half particle is in contact with a cold temperature T_c. The energy level is lowered from D to A according to a certain parameter (such as magnetic field) during a time interval of duration n'. Both work and heat are exchanged during this process. In a similar way calculating the heat released during isothermal compression dividing it in to three adiabatic compression and isochoric process.

i.e,

$Q_{out} = \Delta Q^4 + \Delta Q^5 + \Delta Q^6$.

First step of heat released is from point D to 6

$$\Delta Q^4 = (E_e^D - E_g^D)(p_e^6 - p_e^D), \tag{3.7}$$

in the second step it will release

$$\Delta Q^5 = (E_e^7 - E_g^7)(p_e^8 - p_e^7), \tag{3.8}$$

and in the last step it will release

$$\Delta Q^6 = (E_e^9 - E_g^9)(p_e^{10} - p_e^9). \tag{3.9}$$

The total heat released during isothermal compression is

$$Q_{out} = \Delta Q^4 + \Delta Q^5 + \Delta Q^6. \tag{3.10}$$

Simplifying this with $(p_e^{10} = p_e^B)$, $(p_e^8 = p_e^9)$, $(p_e^7 = p_e^6)$, and $(p_e^D = p_e^C)$;

$$Q_{out} = (E_e^A - E_g^A)p_e^B - (E_e^D - E_g^D)p_e^C + \Delta(p_e^6 + p_e^8 + p_e^B). \tag{3.11}$$

The total work of the engine is the sum of the work on each branch (W_{cyc}=-(W_{AB}+W_{BC}+W_{CD}+W_{DA})). The negative sign is due to the convention of positive W when work is done on the system, which is equivalent to the sum of the absorbed and released heat energies,

$$W_{cyc} = Q_{In} + Q_{out}. \tag{3.12}$$

$$W_{cyc} = \left[1 - \frac{E_e^D - E_g^D}{E_e^C - E_g^C}\right] p_e^C (E_e^C - E_g^C) - \left[1 - \frac{E_e^A - E_g^A}{E_e^B - E_g^B}\right] p_e^B (E_e^B - E_g^B) + \Delta[(p_e^B + p_e^8 + p_e^6) - (p_e^C - p_e^2 - p_e^4)], \tag{3.13}$$

but (p_e^2=p_e^8, p_e^4=p_e^6), there fore the total work done is

$$W_{cyc} = \left[1 - \frac{E_e^D - E_g^D}{E_e^C - E_g^C}\right] p_e^C (E_e^C - E_g^C) - \left[1 - \frac{E_e^A - E_g^A}{E_e^B - E_g^B}\right] p_e^B (E_e^B - E_g^B) + \Delta[(p_e^B - (p_e^C)]. \tag{3.14}$$

As we know, $(1 - \frac{E_e^D - E_g^D}{E_e^C - E_g^C}) = \eta_c = (1 - \frac{E_e^A - E_g^A}{E_e^B - E_g^B})$,

Therefore, the total work in one cycle can be written as

$$W_{cyc} = \eta_c[\Delta_C p_e^C - \Delta_B p_e^B] + \Delta(p_e^B - p_e^C). \tag{3.15}$$

Δ is the energy difference between the consecutive energy spacing[9] which can be written as

$$\Delta = \frac{\Delta_C - \Delta_B}{N}. \tag{3.16}$$

And the efficiency will be

$$\eta = \frac{W_{cyc}}{Q_{In}}. \tag{3.17}$$

3.2 Efficiency at maximum power output

Here our goal is to maximize the power output and to evaluate the corresponding efficiency. We consider the work done and the respective heat transfer for N number of division of the isothermal process. We assume the adiabatic process is completely reversible (no heat exchange with the surrounding) where as in the isothermal process heat is transfer and work is done as we have seen before. From last section Eq(3.15) for N division of the isothermal expansion (compression) the work done is

$$W_{cyc} = \eta_c[\Delta_C p_e^C - \Delta_B p_e^B] + \Delta(p_e^B - p_e^C). \tag{3.18}$$

And the heat absorbed as it expand isothermally will be

$$Q_{In} = (E_e^C - E_g^C)p_e^C - (E_e^B - E_g^B)p_e^B - \Delta(p_e^C + p_e^2 + p_e^4). \tag{3.19}$$

The power output becomes

$$P = \frac{W}{t}. \tag{3.20}$$

Because the time taken for adiabatic expansion and compression process is much smaller as compared to isothermal process we can approximate the time taken for the one cycle as

$$t = n + n', \tag{3.21}$$

where n and n' are the for isothermal expansion and compression and they are nearly equal so $t = 2n$ using Eq(3.20)

$$P = \frac{\eta_c(\Delta_C p_e^C - \Delta_B p_e^B)}{t} + \frac{2(\Delta_C - \Delta_B)(p_e^B - p_e^C)}{t^2}. \tag{3.22}$$

To find the maximum power efficiency first maximize the power output in-terms of the time t.

i.e,

$$\frac{\partial P}{\partial t} \mid_{t_{maxP}} = 0, \tag{3.23}$$

where, t_{maxP} is the time taken at maximum power out put. By using Eqs(3.22), and (3.23) we can get:

$$t_{maxP} = \frac{4(\Delta_C - \Delta_B)(p_e^B - p_e^C)}{\eta_c(\Delta_B p_e^B - \Delta_C p_e^C)}. \tag{3.24}$$

There fore the maximum power efficiency η_{maxP} is calculated as

$$\eta_{maxP} = \frac{W_{(t_{maxP})}}{Q_{In_{(t_{maxP})}}}. \tag{3.25}$$

By substituting Eqs(3.18), (3.19) and (3.24) into Eq(3.25) we get

$$\eta_{maxP} = \frac{\eta_c}{2} + \vartheta(\eta_c). \tag{3.26}$$

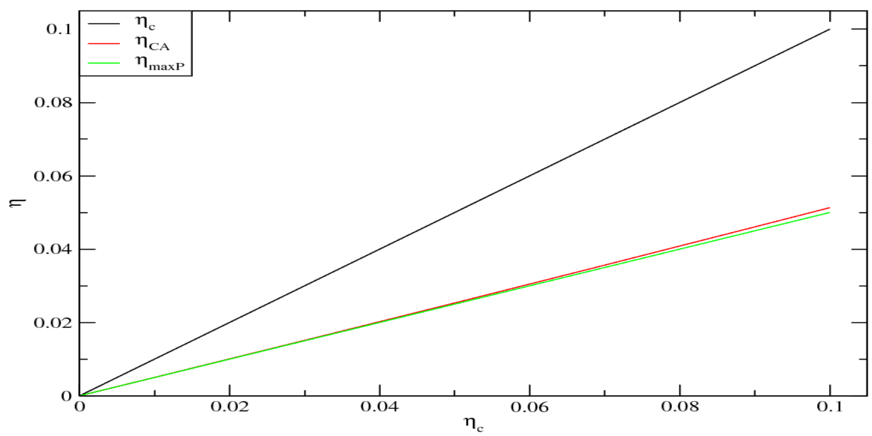


Figure 3.2: Plot of Efficiency at maximum power (green line) compared with Carnot efficiency (black line) and Curzon Ahlborn efficiency (red line) versus Carnot efficiency

Chapter 4

Optimization method using objective function and Optimized efficiency

4.1 Optimization method using objective function

Finite time thermodynamics mainly deals with finding the pathway which yields the optimum performance of finite-size devices at finite-time processes. To achieve this goal, an objective function that depends on parameters of the model must be optimized. In principle one has the freedom of choice of such objective function. However, that a thermodynamic criterion devoted to analyze the optimum regime of operation in a real process should meet the following requirements:

1. its dependence on the parameters of the process should be a guidance in order to improve the performance of that process
2. it should not depend on parameters of the environment, and
3. it should take into account the unavoidable dissipation of energy provoked by the process

There are two widely used ways in optimization of traditional thermodynamics heat devices:

1. The entropy generation minimization and,
2. Exergy analysis.

Both methods are based on the Gouy-Stodola theorem [10], which quantifies the lost available work (or exergy destruction), $W_{lost}= T_o S_{gen}$, for any system operating under irreversible (finite-time) conditions in terms of the corresponding entropy generation, S_{gen}, and the environment temperature, T_o. The application of this theorem to a particular design requires the evaluation of S_{gen} through a model linking the thermodynamic non-ideality of the design to the physical characteristics of the system. However, deriving expressions for S_{gen} is a subtle and, sometimes, difficult task (as it happens for situations where the system is far from the equilibrium). Exergetic methods additionally depend on the parameters of the environment which can be unknown or far from the average values. A number of different optimization criteria have also been proposed, but they suffer from lack of generality since they apply to a particular heat devices, either heat engines, refrigerators, or heat-pump cycles. Although conceptual differences exist between microscopic and macroscopic engines, this facts suggests that the proposed optimization could be used as a unified framework for dealing with molecular and macroscopic engines. Here we use the optimization criteria proposed by Hernandez et.al.[3], which compromises the energy benefits and losses. The requirement set by Hernandez for optimization are the parameters of the process that should be tuned to improve the performance and should not depend on the parameters of the environment. It should take into account the unavoidable dissipation of energy provoked by the process. The conventional efficiency, η, of an energy converter is defined as the ratio between the output energy and input energy:

$$\eta = \frac{E_u(\beta; \{\alpha\})}{E_i(\beta; \{\alpha\})}. \tag{4.1}$$

An energy converter produces a useful energy $E_u(\beta; \{\alpha\})$, for a given input energy

$E_i(\beta;\{\alpha\})$ where β denotes independent parameters while α denotes the set of parameters which can be considered as controls. Let $\eta_{max}\{\alpha\}$ and $\eta_{min}\{\alpha\}$ be the maximum and the minimum efficiencies that can be extracted by our energy converter, respectively. Then, the efficiency $\eta(\beta;\{\alpha\})$, for a particular β and $\{\alpha\}$ should lie in between these two limiting efficiencies;
i.e,

$$\eta_{min}\{\alpha\} \leq \eta(\beta;\{\alpha\}) \leq \eta_{max}\{\alpha\}. \tag{4.2}$$

Substituting Eq.(4.1) into Eq.(4.2) we obtain

$$\eta_{min}\{\alpha\}E_i(\beta;\{\alpha\}) \leq E_u(\beta;\{\alpha\}) \leq \eta_{max}\{\alpha\}E_i(\beta;\{\alpha\}). \tag{4.3}$$

Hernandez et. al. defined two quantities: effective useful energy, $E_{u,eff}(\beta;\{\alpha\})$, as

$$E_{u,eff}(\beta;\{\alpha\}) = E_u(\beta;\{\alpha\}) - \eta_{min}\{\alpha\}E_i(\beta;\{\alpha\}), \tag{4.4}$$

and the lost useful energy, $E_{u,lost}(\beta;\{\alpha\})$, as

$$E_{u,lost}(\beta;\{\alpha\}) = \eta_{max}\{\alpha\}E_i(\beta;\{\alpha\}) - E_u(\beta;\{\alpha\}). \tag{4.5}$$

To evaluate the best compromise between useful energy and lost useful energy they introduced the objective function Ω as the difference between these two quantities:

$$\Omega = E_{u,eff}(\beta;\{\alpha\}) - E_{u,lost}(\beta;\{\alpha\}). \tag{4.6}$$

Substituting Eqs.(4.2), (4.3) and (4.1) into Eq.(4.6) we get the expression for Ω as

$$\Omega = [2\eta(\beta;\{\alpha\}) - \eta_{max}\{\alpha\} - \eta_{min}\{\alpha\}]E_i(\beta;\{\alpha\}). \tag{4.7}$$

Eq.(4.7) is the the objective function proposed by Hernandez et. al.[3]. To analyze the mode of operation of any energy converter giving the best compromise between energy benefits and losses. This proposed criterion gives an optimized efficiency that lies between the maximum and minimum efficiencies. For our engine (spin-half particle), the maximum efficiency attainable is that of Carnot efficiency, η_c, which takes practically the longest time possible per cycle. On the other hand, we will consider the minimum efficiency to correspond to the shortest time possible which is the efficiency at maximum power, η_{maxP}, and zero for the other case.

4.2 Optimized efficiency

In this section we find that the optimized efficiency that lies between the maximum efficiency (Carnot efficiency) and the efficiency at maximum power condition by optimizing the objective function with respect to time and the corresponding time taken to complete one cycle. In our case we have defined the objective function

$$\Omega = (2\eta - (\eta_{min} + \eta_{max}))Q_{In}. \tag{4.8}$$

This objective function enable us to analyze the operational mode of our energy converter giving the best compromise between energy benefits and losses. After taking the time derivative of Eq.(4.8) becomes

$$\dot{\Omega} = (\frac{2\dot{W}}{\dot{Q_{In}}} - (\eta_{min} + \eta_{max}))\dot{Q_{In}}. \tag{4.9}$$

Where $\frac{\dot{W}}{\dot{Q_{In}}} = \eta$, after this we optimized the objective function with respect to time t. The objective function takes its optimized value when

$$\frac{\partial\dot{\Omega}}{\partial t}\mid_{t_{opt}} = 0 \tag{4.10}$$

is satisfied. In our case η_{min} is zero or the efficiency at maximum power (η_{maxP}) and η_{max} is the Carnot efficiency (η_c) therefore, we can get two optimized efficiencies. Thus are described in the next two subsections.

4.2.1 Optimized efficiency when we take zero as the minimum efficiency

In this case Eq.(4.9) can be written as

$$\dot{\Omega} = (\frac{2\dot{W}}{\dot{Q}_{In}} - \eta_c)\dot{Q}_{In}. \qquad (4.11)$$

To calculate the optimized power (P_{opt}), optimized efficiency (η_{opt}), and the corresponding time taken to complete one cycle (t_{opt}), we optimized the objective function with respect to time t. That is

$$\frac{\partial \dot{\Omega}}{\partial t} |_{t_{opt}} = 0. \qquad (4.12)$$

By using Eqs.(3.18), (3.19) and (4.11) into Eq.(4.12) we get

$$t_{opt} = \frac{4(\Delta_C - \Delta_B)[2(p_e^B - p_e^C) + \eta_c(p_e^C + p_e^2 + p_e^4)]}{\eta_c(\Delta_B p_e^B - \Delta_C p_e^C)}. \qquad (4.13)$$

The optimized power efficiency is the ratio of out put optimized power to the in put optimized power, which is

$$\eta_{opt} = \frac{\frac{W}{t_{opt}}}{\frac{Q_{In}}{t_{opt}}} \qquad (4.14)$$

where $\frac{W}{t_{opt}}$=P_{opt}. Using Eqs.(3.18 ; 3.19 and 4.13) into Eq.(4.14) we get the optimized efficiency as

$$\eta_{opt} = \frac{3\eta_c}{4}(1 - \frac{\eta_c x}{12} - \frac{7{\eta_c}^2 x^2}{32} - \ldots) \qquad (4.15)$$

$x = \frac{(p_e^C + p_e^2 + p_e^4)}{(p_e^B - p_e^C)}$, for small Carnot efficiency we can take only the first term, which is:

$$\eta_{opt} = \frac{3\eta_c}{4}. \qquad (4.16)$$

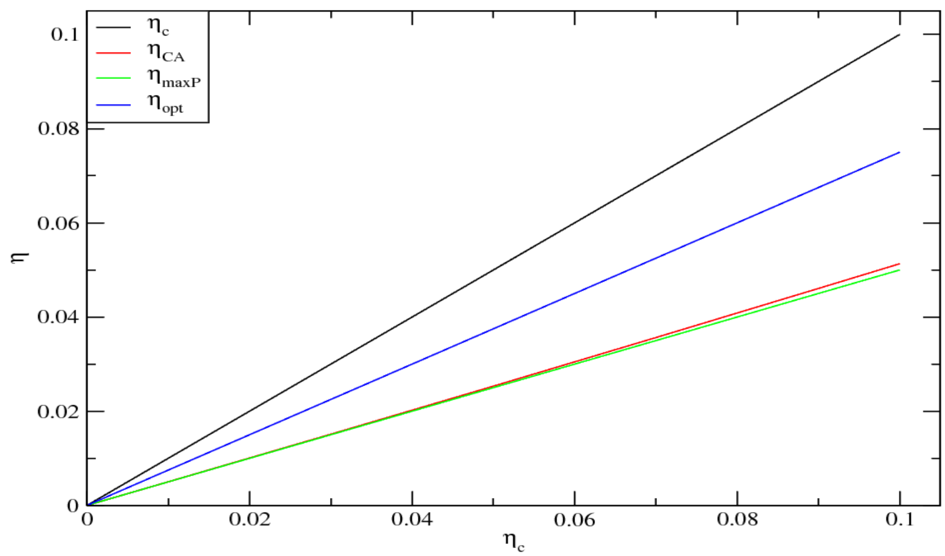


Figure 4.1: Plot of Efficiency at maximum power (green line); at optimized power efficiency when ($\eta_{min} = 0$) (blue line); at Carnot efficiency (black) and Curzon Ahlborn efficiency (red line) versus Carnot efficiency

4.2.2 Optimized efficiency when we take maximum power efficiency as the minimum efficiency

Eq.(4.9) becomes

$$\dot{\Omega} = (\frac{2\dot{W}}{\dot{Q_{In}}} - (\eta_c + \frac{\eta_c}{2}))\dot{Q_{In}}. \quad (4.17)$$

By using the same method as section (4.2.1), we obtain the optimized time taken to complete one cycle of the process, $t_{opt'}$, and the optimized efficiency, $\eta_{opt'}$, as:

$$t_{opt'} = \frac{4(\Delta_C - \Delta_B)[4(p_e^B - p_e^C) + 3\eta_c(p_e^C + p_e^2 + p_e^4)]}{\eta_c(\Delta_B p_e^B - \Delta_C p_e^C)}. \quad (4.18)$$

$$\eta_{opt'} = \frac{\frac{W}{t_{opt'}}}{\frac{Q_{In}}{t_{opt'}}}. \quad (4.19)$$

Using Eqs.(3.18 ; 3.19 and 4.18) into Eq.(4.19), we get the optimized efficiency as

$$\eta_{opt'} = \frac{7\eta_c}{8}[1 - \frac{\eta_c x}{56} - \frac{47{\eta_c}^2 x^2}{128} - \ldots]. \quad (4.20)$$

For small Carnot efficiency we can take only the first term. Which is:

$$\eta_{opt'} = \frac{7\eta_c}{8}. \tag{4.21}$$

Here we use prime (') to differentiate the two optimized values.

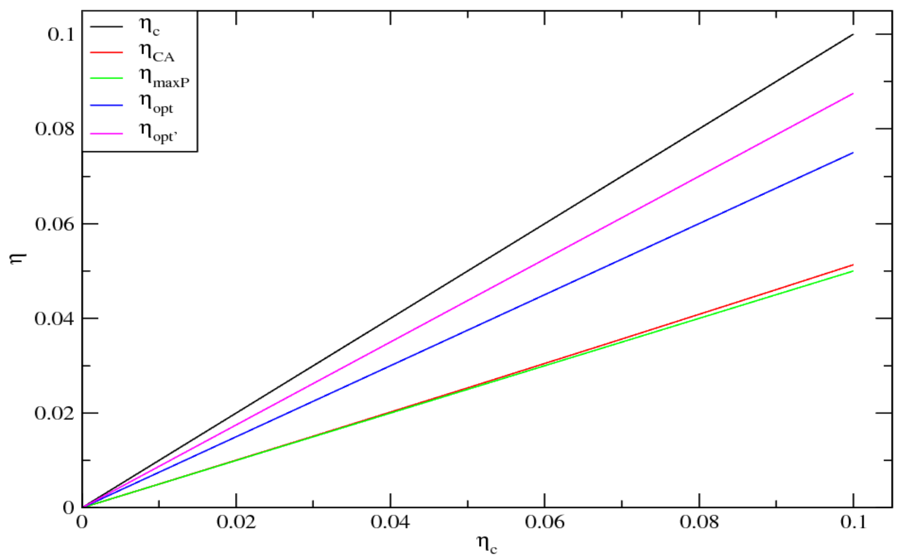


Figure 4.2: Plot of Efficiency at maximum power (green line); at optimized power efficiency when ($\eta_{min} = 0$) (blue line);at optimized power efficiency when ($\eta_{min} = \eta_{maxP}$) (magenta line) at Carnot efficiency (black line) and Curzon Ahlborn efficiency (red line) versus Carnot efficiency.

Fig(4.1 and 4.2) shows that all the efficiencies increase as η_c increase. This is because as we increase η_c the temperature difference of the reservoirs increase. From this we can observe that the work extracted at Carnot cycle more than work extracted at optimized efficiency process which is greater than work extracted from Curzon and Ahlborn cycle process and from work extracted from maximum power efficiency. But the time taken to extract work at one complete cycle of Carnot process is much greater than all other process, and the time taken to extract work at maximum power the fastest of all the others for one complete cycle. This is because at Carnot cycle process there is no dissipation of energy but there is an energy dissipation at the process of optimized efficiency and there is more energy dissipation at the efficiency of maximum power process. We can therefore say that the operation of the spin-half particle at optimized efficiency is indeed a compromise between energy benefits and losses. Since the graph of the optimized power efficiency lies between Carnot efficiency and maximum power efficiency and Curzon and Ahlborn efficiency.

Even if both optimized efficiencies are in between maximum power efficiency and Carnot efficiency but there is more energy dissipation or less time consumption when we use zero minimum efficiency instead of maximum power efficiency as the minimum efficiency.

Chapter 5

Summary and Conclusion

In this work, we consider a spin-half particle with two energy level as a heat engine inside of a magnetic field and embedded between two heat reservoirs. The magnetic field in our model uses to increase the out put work. The simplicity of the model enabled us to get analytic solution for the important quantities such as optimized power, optimized efficiency and the time taken to complete one cycle.

After we calculated the efficiency at maximum power and the corresponding time taken to complete one cycle for our model of spin-half particle as heat engine embedded by heat reservoirs and by magnetic field, we introduce an objective function based on the proposal of Hernandez et.al.[3]. Using optimization principle we optimized the objective function with respect to, t, and we found the point at which the objective function is maximum. We found the optimized efficiency to be exactly $\frac{3\eta_c}{4}$ for zero minimum efficiency and $\frac{7\eta_c}{8}$ for the case when we take maximum power efficiency as minimum efficiency. We also calculated the corresponding optimized time taken to complete one cycle. After this we compared efficiencies: Carnot efficiency, Curzon and Ahlborn, efficiency at maximum power, and optimized efficiency. Carnot efficiency which is the maximum efficiency but it takes in finite time to extract certain amount of work. Hence the corresponding power is zero (finite work divided by infinite time). So for practical application the Carnot efficiency has a limited significance. Curzon and Ahlborn [2] efficiency at nonzero power in a finite time but there is dissipation (wastage) of high amount of heat. Efficiency at maximum power which is nearly the same as Curzon and Ahlborn efficiency as we observe from the graphs for linear regime. Finally, we have optimized efficiency which lies between Curzon and Ahlborn efficiency and Carnot efficiency which tells us it is the best compromise between useful energy and lost energy. But the time taken to complete one cycle at optimized efficiency is greater than that of the fastest time (the time taken to complete one cycle at maximum power).

In general, we believe that our work has, for the first time, found an efficiency which is between the efficiency at maximum power (and also Curzon and Ahlborn [2]) and maximum efficiency (Carnot efficiency) analytically, when the spin-half particle is inside the magnetic field and it is in contact with the heat reservoirs at different temperatures.

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DECLARATION

I hereby declare that this thesis is my original work and has not been presented for a degree in any other university. All sources of material used for the thesis have been duly acknowledged.

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Place and time of submission: Addis Ababa University, November 2011

This thesis has been submitted for examination with my approval as University advisor.

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