OPTIMIZED EFFICIENCY OF A STOCHASTICALLY DRIVEN QUANTUM DOT HEAT ENGINE

Yigermal Bassie Yassabie

A THESIS SUBMITTED TO THE DEPARTMENT OF PHYSICS
PRESENTED IN PARTIAL FULFILLMENT OF THE
REQUIREMENTS FOR THE DEGREE OF
MASTER OF SCIENCE (PHYSICS)

ADDIS ABABA UNIVERSITY
ADDIS ABABA, ETHIOPIA
JUNE 2012

ADDIS ABABA UNIVERSITY
DEPARTMENT OF
PHYSICS

Supervisor: _____
Dr.Mulugeta Bekele

Examiners: _____
Dr. Tatek Yergou

_____
Dr. Lemmi Demeyu

ADDIS ABABA UNIVERSITY

Date: **June 2012**

Author: **Yigermal Bassie Yassabie**

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Department: **Physics**

Degree: **M.Sc.** Convocation: **June** Year: **2012**

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Signature of Author

To

my grandfather Amera Bireku

and

my brother Ayele Dessie

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Abstract

In this thesis, we take a stochastically driven single level quantum dot embedded between two metallic leads at different temperatures which works as a heat engine. We analytically study the optimized efficiency that lies between the maximum efficiency and minimum efficiencies (efficiency at maximum power and the minimum efficiency) condition. We perform two ways of optimization criteria to find their corresponding optimized efficiencies, powers and periods. We study the performance of the heat engine by introducinng a figure of merit as a function of Carnot efficiency.

Acknowledgements

First of all, I would like to thank almighty God who made it possible, to begin and finish this work successfully. I do not have adequate words to express my feelings of gratitude to my advisor and instructor Dr. Mulugeta Bekele, whose benevolent guidance and constant encouragement helped me to complete the present thesis work sucessfully. He is the person who has always helped me as friendly approach and fatherhood advice. I have learned a lot not only in the physics part but also to be kind, patient, respectful and to have confidence in my work. I am very grateful once again to him for all the things he has done for me.

Words can not express my felling which I have for my mother Bizuayhu Amera, my father Bassie Yassabie, Melkamu Amera and whole family. I am highly indebted to them for their blessing, guidance, advice, encouragenment and support.

I would like to convey my special thanks to my friends, Tibebe, Tadle, Anley, Fitsum, Tolasa, Endale, Andargachew and many other for their constant encouragement and help.

I am very happy to thank the International Program in Physical Sciences (IPPS), Uppsala University, Uppsala, Sweden for providing research facilities to our Lab.

Finally I would like to thank the department of physics and school of graduate studies, AAU, MOE, for all support I got during my study.

Chapter 1

Introduction

Thermodynamics is the area of physics that study 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). Thermodynamics laws which govern them originate from very ordinary experiences in our daily lives. In the development of the Second Law of thermodynamics, it is very convenient to have a hypothetical body with a relatively large thermal energy capacity that can supply or absorb finite amounts of heat without undergoing significant change in its energy. We call such a body a 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 thermodynamics, a heat engine is a system that performs the conversions of heat or thermal energy to mechanical work. It does this by bringing a working substance from a high temperature state to a lower temperature state. A heat source generates thermal energy that brings the working substance to the high temperature state. The working substance generates work in the working body of the engine while transfering heat to the cold sink until it reaches a low temperature state. During this process some of the thermal energy is converted into work by exploiting properties of the working substance. The working substance can be any system with a non-zero heat capacity. But it usually is a gas or a liquid.

Work can be converted to heat directly and completely in Joules experiment, 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.

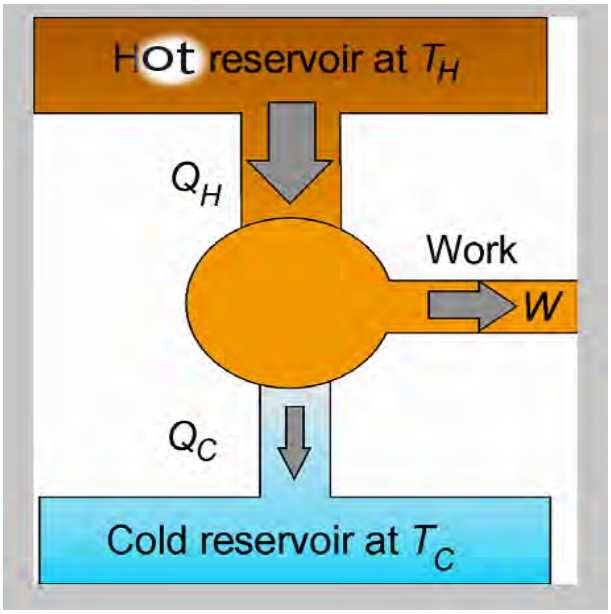

Figure 1.1: Schematic representation of a heat engine

As we see from the above diagram (Fig.1.1), the engine absorbs a quantity of heat energy Q_H from the hot reservoir, does work W, and then gives off a quantity of heat 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

The efficiency of the heat engine is defined as the ratio of the useful work, W, extracted to the heat taken from the hot reservoir, Q_H, i.e

$$\eta = \frac{W}{Q_H} = 1 - \frac{Q_C}{Q_H}. \tag{1.0.1}$$

The concept of Carnot efficiency is a central cornerstone of thermodynamics [1,2]. The

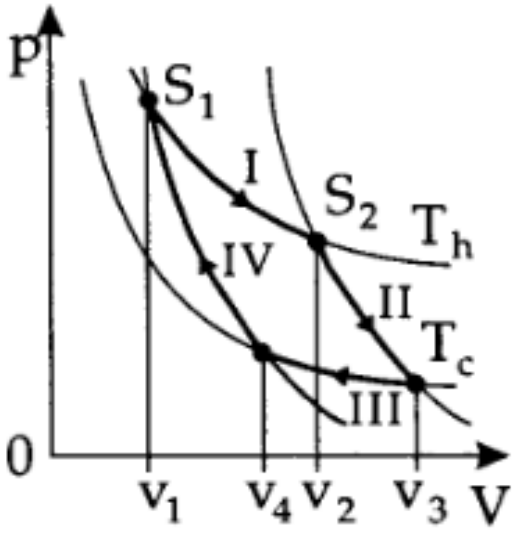

Figure 1.2: Carnot process in the PV diagram

Carnot cycle, with a monoatomic ideal gas as the working material, was presented by Carnot in 1824 [3,4]. The Carnot process is performed in four successive reversible steps, which we will illustrate in a PV diagram (Fig.1.2).

Step 1: Isothermal expansion from volume V_1 to volume V_2 at constant temperature T_H. For this isothermal expansion, we find from the ideal gas equation that

$$\frac{V_2}{V_1} = \frac{P_1}{P_2}. \tag{1.0.2}$$

The internal energy of an ideal gas can not be changed at constant themperature. Consequently the heat absorbed, ΔQ_1, by the gas is

$$\Delta Q_1 = \Delta W_1 = N k_B T_H \ln \frac{V_2}{V_1}, \tag{1.0.3}$$

where N is the number of gas molecules in the container and k_B is Boltzmann's constant. This is the amount of heat exchanged with the heat bath in the first step. Since $V_2 > V_1$, $\Delta Q_1 > 0$; i.e., the amount of heat ΔQ_1 is added to the gas at the expense of the heat bath.

Step 2: Adiabatic expansion of the isolated working material from V_2 to V_3. Here the temperature changes from T_H to T_C. The indices H and C denote hot and cold, so that $T_H > T_C$. Under the adiabatic expansion, the volume (V_2 and V_3) at the ends are related to the temperatures (T_H and T_C) by

$$\frac{V_3}{V_2} = (\frac{T_H}{T_C})^{\frac{3}{2}}. \tag{1.0.4}$$

Since $\Delta Q_2 = 0$ (for Adiabatic process) the work performed in the expansion is taken from the internal energy,

$$\Delta W_2 = -\Delta U_2 = C_v(T_H - T_C). \tag{1.0.5}$$

For an ideal gas C_v is a constant independent of themperature and volume.

Step 3: We now compress the system isothermally from V_3 to V_4 at the constant themperature T_C. Analogous to step 1, we have

$$\frac{V_4}{V_3} = \frac{P_3}{P_4}. \tag{1.0.6}$$

The work ΔW_3 performed during this isothermal compression is released to the heat bath in the form of heat such that

$$\Delta Q_3 = \Delta W_3 = N k_B T_C \ln \frac{V_4}{V_3}. \tag{1.0.7}$$

This is the amount of heat absorbed by the heat bath in this step. Since $V_4 < V_3$, it follows that $\Delta Q_3 < 0$; i.e., the gas loses this amount of heat.

Step 4: Finally we restore the system to the intial state via an adiabatic compresion from V_4 to V_1. During this process the temperature increases from T_C to T_H:

$$\frac{V_1}{V_4} = (\frac{T_C}{T_H})^{\frac{3}{2}}. \tag{1.0.8}$$

Since $\Delta Q_4 = 0$ it follows that

$$\Delta W_4 = -\Delta U_4 = C_v(T_C - T_H). \tag{1.0.9}$$

We now consider the total energy balance of the cyclic process

$$\Delta U_{total} = \Delta Q_1 - \Delta W_1 - \Delta W_2 + \Delta Q_3 - \Delta W_3 - \Delta W_4. \tag{1.0.10}$$

If we insert Eqs. (1.0.3), (1.0.5), (1.0.7), and (1.0.9), we immediately recognize that indeed $\Delta U_{total} = 0$, as it should be for a cycle. We have $\Delta Q_1 - \Delta W_1 = 0$ and $\Delta Q_3 - \Delta W_3 = 0$ and further more $\Delta W_2 = -\Delta W_4$. From Eq.(1.0.4) and Eq.(1.0.8) we get

$$\frac{V_1}{V_2} = \frac{V_4}{V_3}. \tag{1.0.11}$$

The Carnot process effectively performs a work ΔW that is

$$\Delta W = \Delta W_1 + \Delta W_2 + \Delta W_3 + \Delta W_4 = Nk_BT_H \ln\frac{V_2}{V_1} + Nk_BT_C \ln\frac{V_4}{V_3}$$
$$\Delta W = Nk_B(T_H - T_C)\ln\frac{V_2}{V_1}. \tag{1.0.12}$$

Since $T_H > T_C$ and $V_1 < V_2$, this is a positive quantity. Hence ΔW is work performed by the gas in one cycle. Obviously, a Carnot engine is an engine which transforms part of its intake heat into work. The work performed by the engine increases with the temprature difference and with the compression ratio $\frac{V_2}{V_1}$. Based on Eq.(1.0.1) the efficiency of this engine is

$$\eta_C = \frac{\Delta W}{\Delta Q_1} = 1 - \frac{T_C}{T_H}. \tag{1.0.13}$$

From thermodynamic point of view this efficiency increases as Tc decreases. In other words, the lower the temperature of the cold system (to which heat is delivered), the

higher the engine efficiency for fixed T_H. The maximum possible efficiency, $\eta_C = 1$, occurs if the temperature of the cold source is equal to zero and the temperature of the hot source is nonzero. If a reservoir at zero temperature were available as a heat repository, heat could be freely and completely converted into work. However, such heat repository is no available in the world [5].

The Second Law of thermodynamics puts a fundamental limit on the thermal efficiency of all heat engines. Surprisigly, even ideal, frictionless engine can not convert all the input energy into work.

The practical implications of Carnot efficiency is limited since it is 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 maximum, the output power is zero.

Practically we need to operate the heat engines in a finite time to obtain a finite power. Curzon and Ahlborn [6] considered a phenomenological model of a finite-time Carnot heat engine under the assumptions that heat flow obeys the linear Fourier law and that irreversibility occurs only due to the heat flow (endoreversible approximation) [5,6], and they obtained the efficiency η_{CA} , at maximum power to be

$$\eta_{CA} = 1 - \sqrt{\frac{T_C}{T_H}}. \tag{1.0.14}$$

Operating at maximum power, however, wastes a large amount of the input energy though the task is accomplished in a short enough time. One can think of minimizing the wastage by appropriately relaxing the operating time and, hence, optimizing the efficiency of the device.

Optimization finds the pathway that yields optimum performance in a process operating at nonzero rates. For macroscopic heat engines and refrigerators different optimization techniques had been developed and applied to optimize the efficiency and coefficient of performance. Hernandez *et.al.* [7] came up with unified optimization criteria which works for both macroscopic and microscopic energy converters. According to there proposed

criteria the optimized efficiency lies between the maximum and minimum efficiencies .

In this thesis work we will consider a model that consists of a single level quantum dot in contact with hot and cold heat reservoirs proposed by M. Esposito *et.al.* [8]. This recently proposed model is composed of a quantum dot embedded between two metallic leads at different temperatures and chemical potentials. They studied how the device operates as a heat engine (quantum dot embedded between two metallic leads at different temperatures and similar chemical potentials) and determined the efficiency at maximum power and compared theire value with that of the Curzon-Alhborn efficiency.

The main purpose of this work is to find exact expression for an optimum efficiency and the corresponding time taken to complete one cycle when a stochastically driven single level quantum dot embedded between two metallic leads at different temperatures and the same chemical potentials operate as a heat engine.

The rest of the thesis is organized as follows. In Chapter 2, we present the model as studied by M. Esposito *et.al.* [8]. In Chapter 3, we describe the method of optimization criteria proposed by Hernandez *et.al.* [7]. An important feature of this proposed criterion is that it gives an optimized efficiency that lies between the maximum efficiency and minimum efficiencies (efficiency at maximum power condition and the minimum efficiency). In Chapter 4, by using optimization criteria we optimize the objective function with respect to two free parameters, and then we calculate and study the optimized efficiencies of the model, the period, the power and the figure of merit as a function of Carnot efficeincy, η_C. Finally Chapter 5 deals with summary and conclusion.

Chapter 2

Efficiency at maximum power

In this Chapter we go through the work of M.Esposito *et.al* [8] as a starting point of consideration for our model. M.Esposito *et.al* [8] consider a stochastically driven single level quantum dot in contact between two (hot and cold) heat reservoires with the same chemical potential and following their analysis we drive the thermodynamics quantities such as heat flux, current, power, entropy and efficiency.

2.1 Stochastically driven single level quantum dot: a nano-scale finite-time thermodynamic machine

Quantum dots are semiconductor nanocrystals that are so small and considered as dimensionless. Quantum dots range from 2-10 nanometers (10-50 atoms) in diameter [9]. Quantum Dots are more closely related to atoms than a bulk material because of their discrete, quantized energy levels. Quantum dots can be synthesized from a variety of materials, and are primarily made from the III-V and II-VI class of semiconductors. These include gallium arsenide, indium phosphide, indium arsenide, cadmiumselenide, and zinc sulfide.

On the nano-scale, when the electron is confined, the change in energy levels becomes distinctly discrete a condition known as quantum confinement, hence the bandgap is a

function of size. When the quantum dot becomes smaller and smaller the band gap becomes larger and larger.Then height, and energy difference, between energy levels increases as the size of the quantum dot decreases.

2.1.1 Model and dynamics

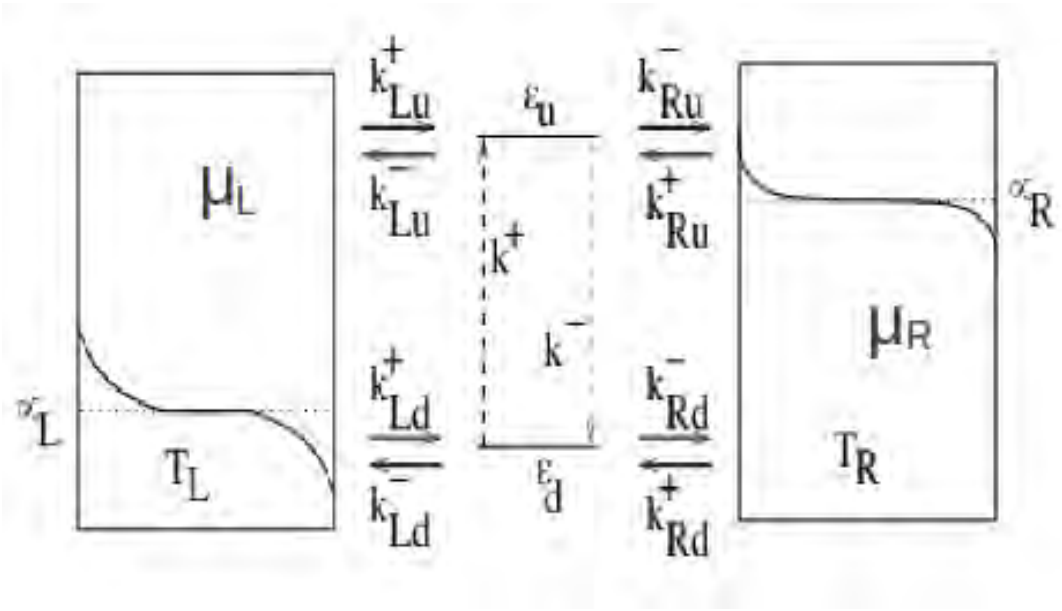

Figure 2.1: The model consists of a single level quantum dot. A stochastic external force causes the energy of the dot to undergo transitions between two values, $\epsilon_u \geq \epsilon_d$, at random times with rates k^+ and k^-.The dot also exchanges electrons with two leads that may be at different chemical potentials μ_L and μ_R and temperatures T_L and T_R [8].

We consider a single-level quantum dot whose energy is stochastically switched between an upper and a lower value, ϵ_j with j = u, d. The upward and downward rates are k^+ and k^-. The dot is in contact with a left and a right lead, ν = L, R, at chemical potentials μ_ν and temperatures T_ν . The transition rates of an electron into lead ν from the dot, and out of lead ν to the dot, are given respectively by $k^-_{\nu j}$= $\Gamma_{\nu j}(1 - f_{\nu j}$) and $k^+_{\nu j}$= $\Gamma_{\nu j} f_{\nu j}$. Here

$$f_{\nu j} = \frac{1}{1 + e^{\frac{\epsilon_j - \mu_\nu}{T_\nu}}} \tag{2.1.1}$$

is the Fermi distribution in lead ν, and $\Gamma_{\nu j}$ is the coupling strength between this lead and

the dot in state j.

The four possible states of the system are denoted by $\{u1, u0, d1, d0\}$, where jn defines whether the level $j = u, d$ is empty or occupied, $n = 0, 1$. The Markovian master equation for the evolution of the state occupation probabilities in terms of $k_j^{\pm} \equiv k_{Lj}^{\pm} + k_{Rj}^{\pm}$ the total transition rate out of the dot (+) or into the dot (-) of either lead, is given by

$$\begin{bmatrix} \dot{P}_{u1} \\ \dot{P}_{u0} \\ \dot{P}_{d1} \\ \dot{P}_{d0} \end{bmatrix} = \begin{bmatrix} -(k^- + k_u^-) & k_u^+ & k^+ & 0 \\ k_u^- & -(k^- + k_u^-) & 0 & k^+ \\ k^- & 0 & -(k^+ + k_d^-) & k_d^+ \\ 0 & k^- & k_d^- & -(k^+ + k_d^+) \end{bmatrix} \begin{bmatrix} P_{u1} \\ P_{u0} \\ P_{d1} \\ P_{d0} \end{bmatrix} \tag{2.1.2}$$

The probability currents between the four states are

$$I_{un} \leftarrow_{dn} = k^+ P_{dn} - k^- P_{un} \tag{2.1.3}$$

for $n = 0, 1$, and

$$I_{j1}^{(\nu)} \leftarrow_{j0} = k_{\nu j}^+ P_{j0} - k_{\nu j}^- P_{j1} \tag{2.1.4}$$

for $j = u, d$. It is convenient to introduce the total current to the quantum dot when it is down or up, that is, the sum, $I_{j1} \leftarrow_{j0} = \sum_\nu I_{j1}^{(\nu)} \leftarrow_{j0}$. Using Eq.(2.1.2) we easily verify that at steady state there is the appropriate balance between the currents, that is,

$$I \equiv I_{u1} \leftarrow_{d1} = -I_{u0} \leftarrow_{d0} = -I_{u1} \leftarrow_{u0} = I_{d1} \leftarrow_{d0} . \tag{2.1.5}$$

The steady state probabilities can be obtained analytically (not shown here) and lead to the following expressions for the current:

$$I = (\frac{k^+ k^-}{k^+ + k^-}) \frac{\sum_\nu \Gamma_{\nu u}(\Gamma_{Ld} f_{Ld} + \Gamma_{Rd} f_{Rd} - \Gamma_d f_{\nu u})}{k^- \Gamma_d + k^+ \Gamma_u + \Gamma_d \Gamma_u},$$

$$I_{d1}^{(L)} \leftarrow_{d0} = (\frac{k^- \Gamma_{ld}}{k^+ + k^-})[\frac{(k^- + \Gamma_u)\Gamma_{Rd}(f_{Ld} - f_{Rd})}{k_- \Gamma_d + k_+(\Gamma_u \Gamma_d \Gamma_u} + \frac{k_+(\Gamma_u f_{ld} - \Gamma_{lu} f_{lu} + \Gamma_{Ru} f_{RU}}{k_- \Gamma_d + k_+(\Gamma_u \Gamma_d \Gamma_u}]. \tag{2.1.6}$$

We have introduced the combination $\Gamma_d \equiv \Gamma_{Ld} + \Gamma_{Rd}$, and similarly for Γ_u. $I_{u1}^{(L)} \leftarrow_{u0}$ is obtained from $I_{d1}^{(L)} \leftarrow_{d0}$ with the substitutions $u \leftrightarrow d$ and $k^+ \leftrightarrow k^-$

2.1.2 Derivation of the thermodynamic quantities

The energy current injected in the system by the stochastic driving reads

$$I_{ext} = (\varepsilon_u - \varepsilon_d) I_{u1} \leftarrow_{d1} = (\varepsilon_u - \varepsilon_d) I, \tag{2.1.7}$$

while the matter (M) and energy (E) currents entering the system from lead ν are given by

$$\begin{aligned} I_M^{(\nu)} &= \sum_j I_{j1}^{(\nu)} \leftarrow_{j0} \\ I_E^{(\nu)} &= \sum_j \varepsilon_j I_{j1}^{(\nu)} \leftarrow_{j0} . \end{aligned} \tag{2.1.8}$$

The heat flux from the lead ν is

$$\dot{Q}^{(\nu)} = I_E^{(\nu)} - \mu_\nu I_M^{(\nu)}. \tag{2.1.9}$$

It is easy to verify matter and energy conservation at steady state to be satisfied respectively.

$$I_M^{(L)} = -I_M^{(R)}$$

and

$$I_{ext} = -I_E^{(L)} - I_E^{(R)}. \tag{2.1.10}$$

As a result power becomes the sum of two contributions,

$$\dot{W} = -\sum_\nu \dot{Q}^{(\nu)} = (\varepsilon_u - \varepsilon_d) I + (\mu_R - \mu_L) I_M^{(L)}. \tag{2.1.11}$$

The first term on the right hand side of Eq.(2.1.11) is the contribution of the energy flux injected by the stochastic driving, while the second term is the energy flux required to bring an electron from the left lead through the dot to the right lead. Since at steady state entropy production, $\dot{S}_i$, is minus the entropy flow, that is,

$$\dot{S}_i = -\sum_\nu \frac{\dot{Q}^{(\nu)}}{T_\nu} \geq 0, \tag{2.1.12}$$

we find that entropy production is the sum of three force-flux terms,

$$\dot{S}_i = (\frac{\varepsilon_u - \varepsilon_d}{T_R})I + (\frac{\mu_L}{T_L} - \frac{\mu_R}{T_R})I_M^{(L)} + (\frac{1}{T_R} - \frac{1}{T_L})I_E^{(L)}. \tag{2.1.13}$$

That is the force of energy flux injected by the stochastic driving, thermodynamics force for matter flow and thermodynamics force for energy flow respectively.

The system reaches equilibrium when entropy production vanish, $\dot{S}_i = 0$, which implies that all currents in the system also vanish. In general, this requires that the three thermodynamic forces vanish separately, i.e., that $\varepsilon_u = \varepsilon_d$, $\mu_L = \mu_R$ and $T_L = T_R$. This is however not necessary when $\Gamma_{Lu}/\Gamma_{Ld} \to 0$ (disallowing transitions from u to L) , and $\Gamma_{Rd}/\Gamma_{Ru} \to 0$ (disallowing transitions from d to R). This combined limit corresponds to a regime of tight coupling, where the transport of matter, energy and heat become proportional to each other because, by removing the possibility of transitions from u to L and from d to R, there is a single pathway connecting the left and right leads. As a result entropy production can be expressed as $\dot{S}_i = XI$, i.e. in terms of the collapsed effective force

$$X = (\frac{\varepsilon_u - \varepsilon_d}{T_R}) + (\frac{\mu_L}{T_L} - \frac{\mu_R}{T_R}) + \varepsilon_d(\frac{1}{T_R} - \frac{1}{T_L}), \tag{2.1.14}$$

and the single flux I

$$I = I_M^{(L)} = \frac{I_E^{(L)}}{\varepsilon_d} = \alpha(f_{Ld} - f_{RU}), \tag{2.1.15}$$

where $\alpha = k^+k^-\Gamma_{Ld}\Gamma_{Ru}/\{(k^+ + k^-)(k^-\Gamma_{Ld} + k^+\Gamma_{Ru} + \Gamma_{Ld}\Gamma_{Ru})\}$. We now see that equilibrium only requires the effective force to vanish, X = 0, without the requirement that the three thermodynamic forces vanish separately.

2.2 Derivation of efficiency at maximum power of the model

We are considering our model under more conventional operating conditions, namely, when the leads are at different temperatures, say $T_L \geq T_R$. For this condition it is

sufficient to consider the simplified case of equal chemical potentials, $\mu = \mu_L = \mu_R$. Entropy production now reads

$$T_R \dot{S}_i = \Delta\varepsilon I + \eta_C \dot{Q}^{(L)} \geq 0, \tag{2.2.1}$$

where $\eta_C = 1 - \frac{T_R}{T_L}$ is the Carnot efficiency. When operating as a heat engine, the machine produces net work on the stochastic driving process, i.e. $I_{ext} \leq 0$, at the cost of a driving heat flow $\dot{Q}^{(L)} \leq 0$. The power output and efficiency of this transformation are given by

$$\begin{aligned} P &= -\Delta\varepsilon I \\ 0 \leq \eta &= \frac{-\Delta\varepsilon I}{\dot{Q}^L} \leq \eta_C. \end{aligned} \tag{2.2.2}$$

In the tight coupling limit, the collapsed force in Eq.(2.1.14) appearing in the entropy production, $\dot{S}_i = XI$, becomes $X = x_R - x_L$ with $x_R = \frac{\varepsilon_u - \mu}{TR}$ and $x_L = \frac{\varepsilon_d - \mu}{TL}$. Here we have used $I_M^{(L)} = I$ and $I_E^{(L)} = \varepsilon_d I$. The efficiency in Eq.(2.2.2) now reduces to

$$\eta = -\frac{\Delta\varepsilon}{\varepsilon_d - \mu} = 1 - \frac{x_R}{x_L}(1 - \eta_C). \tag{2.2.3}$$

Turning to the regime of maximum power in the tight coupling regime, power becames

$$P = -(\varepsilon_u - \varepsilon_d)I = T_L(x_L - x_R)(1 - \eta_C)I(x_L, x_R). \tag{2.2.4}$$

To get the efficiency at maximum power, the output power takes its maximum value when

$$\frac{\partial P}{\partial x_L} \mid_{{x_L}^{mp}} = 0 = \frac{\partial P}{\partial x_R} \mid_{{x_R}^{mp}} \tag{2.2.5}$$

is satisfied.

$$\frac{\partial P}{\partial x_L} \mid_{{x_L}^{mp}} = f_L - f_R + f_L^2 e^{x_L^{mp}}[x_L^{mp} - x_R^{mp}(1 - \eta_c)] = 0. \tag{2.2.6}$$

and

$$\frac{\partial P}{\partial x_R} \mid_{{x_R}^{mp}} = f_L - f_R + f_R^2 e^{x_R^{mp}}[\frac{x_L^{mp}}{1 - \eta_c} - x_R^{mp}] = 0. \tag{2.2.7}$$

Note that in Eq.(2.2.6) and Eq.(2.2.7) the quantities f_L and f_R are for the Fermi distribution evaluated by taking the values for the scaled electron energy barriers at maximum

power $x_{L^{mp}}$ and $x_{R^{mp}}$, respectively. Substract Eq.(2.2.7) from Eq.(2.2.6) we get

$$x_{R^{mp}} = 2\ln[\sqrt{\frac{1}{1-\eta_c}}\cosh(\frac{x_{L^{mp}}}{2}) + \sqrt{\frac{\cosh^2\frac{x_{L^{mp}}}{2}}{1-\eta_c} - 1}] \tag{2.2.8}$$

From Eq.(2.2.6) we get

$$\begin{aligned} x_{L^{mp}} + \sinh(x_{L^{mp}}) + 2(\eta_c - 1)\ln[\sqrt{\frac{1}{1-\eta_c}}\cosh(\frac{x_{L^{mp}}}{2}) + \sqrt{\frac{\cosh^2\frac{x_{L^{mp}}}{2}}{1-\eta_c} - 1}] \\ -\sqrt{2}\cosh(\frac{x_{L^{mp}}}{2})\sqrt{\cosh(x_{L^{mp}}) + 2\eta_c - 1} = 0 \end{aligned} \tag{2.2.9}$$

However an analytical solution of this equation is not possible. Hence, we turn to two cases either find perturbative solution for η_c close to the limiting values of zero, or find numerical solutions for $x_{L^{mp}}$ and $x_{R^{mp}}$ for different values of η_C (for any reservoir temperatures.)

2.2.1 Perturbative solution of efficiency at maximum power

When the temperatures of the left and the right leads are close to each other, the Carnot efficiency becomes very small and we can apply perturbative solution of efficiency at maximum power. Within this range we can expand $x_{L^{mp}}$ in powers of η_c,

$$x_{L^{mp}} = a_0 + a_1\eta_c + a_2\eta_c^2 + \vartheta\eta_c^3. \tag{2.2.10}$$

Using this in Eq.(2.2.9) and expanding the resulting equation in powers of η_c, the coefficients a_o, a_1 and a_2 are found recursively by solving order by order in powers of η_c. Hence we find the coefficients of $x_{L^{mp}}$ to be

$$\begin{aligned} a_0 = &\quad 2.39936 \\ a_1 = &-0.599839 \\ a_2 = &-0.19946 \end{aligned} \tag{2.2.11}$$

Subestitute these value in to Eq.(2.2.10) we get

$$x_{L^{mp}} = 2.39936 - 0.599839\eta_c - 0.19946\eta_c^2 + \vartheta\eta_c^3. \tag{2.2.12}$$

Substitution of these results in Eq.(2.2.8) we get

$$x_{R^{mp}} = 2.39936 + 0.599839\eta_c + 0.400379\eta_c^2 + \vartheta\eta_c^3. \tag{2.2.13}$$

Substitution of these results and Eq.(2.2.13) in Eq.(2.2.3) leads to the solution of the transcendental equation can also be solved perturbatively for small η_c,

$$\eta_{mp} = \frac{\eta_c}{2} + \frac{\eta_c^2}{8} + \vartheta\eta_c^3. \tag{2.2.14}$$

We thus recover the universal value $\frac{\eta_c}{2}$ in the linear regime [4] , as well as the factor 1/8 for the quadratic coefficient [1]. This latter result thus again supports the universality of this value (for systems with a left/right symmetry) and here we can see that the coefficient of the linear ($\frac{1}{2}$) and the quadratic terms ($\frac{1}{8}$) agrees with that of the Curzon-Alhborn model. The corresponding value of the flux at maximum power efficiency of our system becomes

$$I_{mp} = \alpha[\frac{1}{1+e^{x_L^{mp}}} - \frac{1}{1+e^{x_R^{mp}}}]. \tag{2.2.15}$$

The period, τ_{mp}, taken to operate one cycle at maximium power becomes

$$\tau_{mp} \propto \frac{1}{I_{mp}} = \frac{(e^{x_R^{mp}}+1)(e^{x_L^{mp}}+1)}{e^{x_L^{mp}} - e^{x_R^{mp}}}. \tag{2.2.16}$$

2.2.2 Numerical solutions for different values of carnot efficiency

In this subsection we solve for the value of $x_{L^{mp}}$ for different values of η_c numerically. Then we find the corresponding value of $x_{R^{mp}}$ from Eq.(2.2.8). Finally we substitute the values we get for $x_{L^{mp}}$ and $x_{R^{mp}}$ in Eq.(2.2.3) to find the efficiency at maximum power.

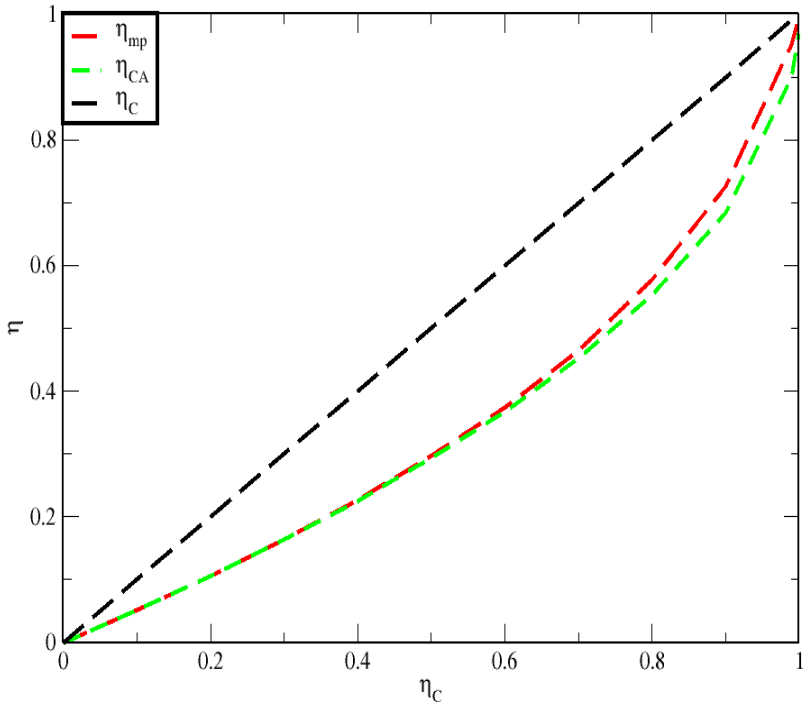

Figure 2.2: Efficiency at maximum power, η_{mp}, for the thermal engine as a function of Carnot efficiency η_C, in comparison with the Curzon-Ahlborn efficiency $\eta_{CA} = 1-\sqrt{1-\eta_C}$

From the Fig.(2.2) which is the numerical solution for the efficiency at maximum power versus Carnot efficiency. We can observe that as Carnot efficiency increases the efficency at maximum power, η_{mp} increases monotonically. It is bounded from the above by carnot efficency, η_C, and lower by the Curzon-Ahlborn efficiency, $\eta_{CA} = 1 - \sqrt{1-\eta_C}$.
Now by using this model as a base in the next two Chapters we are going to introduce the optimization criterion and use it to calculate and study two kinds of optimized efficiencies, periods, powers and the figure of merits of the model as a function of Carnot efficiency.

Chapter 3

Optimization method using objective function

In this Chapter we will introduce an optimization criterion for energy converters which is first introduced by A. Calvo Hernandez *et.al* [7]. This optimization criterion will then be applied to the model we are considering

3.1 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 [10,11] 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.*[7] which compromises the energy benefits and losses. The requirement set by Hernandez *et.al.*[7] 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:

$$\eta = \frac{E_u(x;\{\alpha\})}{E_i(x;\{\alpha\})}. \tag{3.1.1}$$

An energy converter produces a useful energy $E_u(x;\{\alpha\})$, for a given input energy $E_i(x;\{\alpha\})$ where x 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 $\eta(x;\{\alpha\})$, for a particular x and $\{\alpha\}$ should lie in between these two limiting efficiencies;

i.e,

$$\eta_{min}\{\alpha\} \leq \eta(x;\{\alpha\}) \leq \eta_{max}\{\alpha\}. \tag{3.1.2}$$

Substituting Eq.(3.1.1) into Eq.(3.1.2) we obtain

$$\eta_{min}\{\alpha\}E_i(x;\{\alpha\}) \leq E_u(x;\{\alpha\}) \leq \eta_{min}\{\alpha\}E_i(x;\{\alpha\}). \tag{3.1.3}$$

Hernandez *et.al.*[7] to evaluate the best compromise between useful energy and lost useful energy, we introduce the objective function (Ω function) as the difference between these two quantities:

effective useful energy, $E_{u,eff}(x;\{\alpha\})$, as

$$E_{u,eff}(x;\{\alpha\}) = E_u(x;\{\alpha\}) - \eta_{min}\{\alpha\}E_i(x;\{\alpha\}), \tag{3.1.4}$$

and

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

$$E_{u,lost}(x;\{\alpha\}) = \eta_{max}\{\alpha\}E_i(x;\{\alpha\}) - E_u(x;\{\alpha\}). \tag{3.1.5}$$

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:

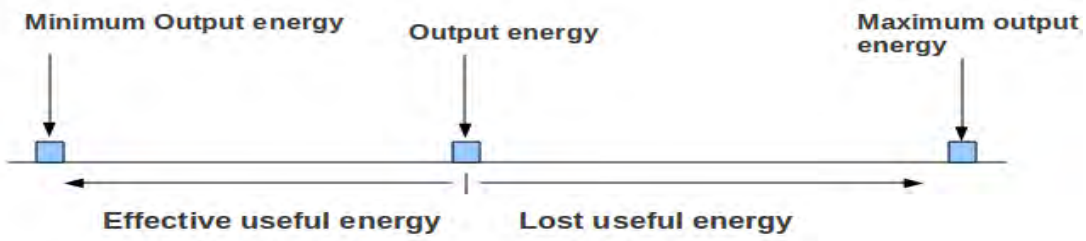

Figure 3.1: schematic representation of the output energy by the stochastic single level quantum dot heat engine under the ranges of effective useful energy and lost useful energy

$$\Omega = E_{u,eff}(x;\{\alpha\}) - E_{u,lost}(x;\{\alpha\}). \tag{3.1.6}$$

Substituting Eq.(3.1.2), Eq.(3.1.3) and Eq.(3.1.1) into Eq.(3.1.6) we get the expression for Ω as

$$\Omega = [2\eta(x;\{\alpha\}) - \eta_{max}\{\alpha\} - \eta_{min}\{\alpha\}]E_i(x;\{\alpha\}). \tag{3.1.7}$$

Eq.(3.1.7) is the the objective function proposed by Hernandez *et.al.*[7]. 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 (stochastically driven single level quantum dot heat engine), 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_{mp} and zero for the athere case.

To optimize the energy converter we use the two quantities defined by Hernandez *et.al.* [7]. The effective useful energy is the difference between useful energy and minimum energy (energy at the poorest efficiency). The other quantity is the lost useful energy which is the difference between the maximum energy (energy at the maximum efficiency)

and the useful energy. These two quantities are functions of independent and dependent parameters describing the process. Using the set of control parameters we optimize the objective function which is the difference between the effective useful energy and the lost useful energy.

Chapter 4

Optimized efficiency

In this Chapter we find that the optimized efficiency that lies between the maximum efficiency(Carnot efficiency) and minimum efficiencies (efficiency at maximum power and the minimum efficiency) condition by optimizing the rate of objective function with respect to the left lead scaled electron energy barriers (x_L) and the right lead scaled electron energy barriers (x_R). In our case we have defined the objective function

$$\Omega = (2\eta - \eta_{min} - \eta_{max})Q_{In}. \tag{4.0.1}$$

This objective function enable us to analyze the operational mode of our energy converter giving the best compromise between energy benefits and losses. We take the time derivative of Eq.(4.0.1) to obtaine

$$\dot{\Omega} = (2\eta - \eta_{min} - \eta_{max})\dot{Q}_{In} \tag{4.0.2}$$

where $\dot{Q}_{In}$=$T_L x_L \alpha(f(x_L) - f(x_R))$.

Then we optimized the rate of objective function with respect to the right lead scaled electron energy barrier and left lead scaled electron energy barrier (x_R and x_L) respectively. The objective function takes its optimized value when

$$\frac{\partial \dot{\Omega}}{\partial x_R} \mid_{x_R{}^{opt}} = 0 = \frac{\partial \dot{\Omega}}{\partial x_L} \mid_{x_L{}^{opt}} \tag{4.0.3}$$

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

4.1 Optimized efficiency when we take minimum efficiency to be zero

In this case Eq.(4.0.2) can be rewritten as

$$\dot{\Omega} = [2(1 - \frac{x_R}{x_L}(1 - \eta_c)) - \eta_c]\alpha T_L x_L (f(x_L) - f(x_R)). \tag{4.1.1}$$

To get the optimized efficiency we first optimize the rate of objective function with respect to x_L and x_R, i,e,

$$\frac{\partial \dot{\Omega}}{\partial x_L} \mid_{x_L{}^{opt}} = f_{L^{opt}} - f_{R^{opt}} - f^2_{L^{opt}} e^{x_L^{opt}} [x_L^{opt} - 2x_R^{opt}(\frac{1-\eta_c}{2-\eta_c})] = 0. \tag{4.1.2}$$

and

$$\frac{\partial \dot{\Omega}}{\partial x_R} \mid_{x_R{}^{opt}} = f_{L^{opt}} - f_{R^{opt}} - f^2_{R^{opt}} e^{x_R^{opt}} [x_R^{opt} - x_L^{opt}(\frac{2-\eta_c}{2\eta_c - 2})] = 0. \tag{4.1.3}$$

Note that in the above expression $f_{L^{opt}}$ and $f_{R^{opt}}$ are the fermi distributions at optimized efficiency. Subtracting Eq.(4.1.2) from Eq.(4.1.3) we find the relationship between x_L^{opt} and x_R^{opt} as

$$\cosh(\frac{x_{R^{opt}}}{2}) = \sqrt{\frac{2-\eta_c}{2\eta_c - 2}} \cosh(\frac{x_{L^{opt}}}{2}). \tag{4.1.4}$$

From the identity of the hyperbolic function we know that

$$\cosh^2(\frac{x_{R^{opt}}}{2}) - \sinh^2(\frac{x_{R^{opt}}}{2}) = 1. \tag{4.1.5}$$

Substituting Eq.(4.1.4) into Eq.(4.1.5) we get

$$\sinh(\frac{x_{R^{opt}}}{2}) = \sqrt{\frac{2-\eta_c}{2\eta_c-2}\cosh^2(\frac{x_{L^{opt}}}{2})-1}. \tag{4.1.6}$$

Adding Eq.(4.1.4) and Eq.(4.1.6) and using the definition of hyperbolic function for $\cosh(\frac{x_{R^{opt}}}{2})$ and $\sinh(\frac{x_{R^{opt}}}{2})$ we get

$$e^{\frac{x_{R^{opt}}}{2}} = \sqrt{\frac{2-\eta_c}{2\eta_c-2}}\cosh(\frac{x_{L^{opt}}}{2}) + \sqrt{\frac{2-\eta_c}{2\eta_c-2}\cosh^2(\frac{x_{L^{opt}}}{2})-1}. \tag{4.1.7}$$

Taking the natural Logarithm of both sides of the above equation the expression for $x_{R^{opt}}$ becames

$$x_{R^{opt}} = 2\ln[\sqrt{\frac{2-\eta_c}{2\eta_c-2}}\cosh(\frac{x_{L^{opt}}}{2}) + \sqrt{\frac{2-\eta_c}{2\eta_c-2}\cosh^2(\frac{x_{L^{opt}}}{2})-1}]. \tag{4.1.8}$$

And rearranging the terms in Eq.(4.1.2) we have

$$x_{L^{opt}} - x_{R^{opt}}[\frac{2-2\eta_c}{2-\eta_c}] + \frac{f_{R^{opt}}}{f^2_{L^{opt}}e^{x_{L^{0pt}}}}^{-}\frac{1}{f_{L^{opt}}e^{x_{L^{opt}}}} = 0. \tag{4.1.9}$$

On the other hand

$$\frac{1}{f_{L^{opt}}e^{x_{L^{opt}}}} = 1+\cosh(x_{L^{opt}}) - \sqrt{\cosh^2(x_{L^{opt}})-1}. \tag{4.1.10}$$

$$\frac{f_{R^{opt}}}{f^2_{L^{opt}}e^{x_{L^{0pt}}}} = 2\cosh^2(\frac{x_{L^{opt}}}{2}) - 2\cosh(\frac{x_{L^{opt}}}{2})\sqrt{\cosh^2(\frac{x_{L^{opt}}}{2}) - \frac{2(1-\eta_c)}{2-\eta_c}}. \tag{4.1.11}$$

Substituting Eqs.(4.1.8), (4.1.10) and (4.1.11) in to (4.1.9) we get

$$x_{L^{opt}} + \frac{4(\eta_c-1)}{2-\eta_c}\ln[\sqrt{\frac{2-\eta_c}{2(1-\eta_c)}\cosh(\frac{x_{L^{opt}}}{2})} + \sqrt{\frac{2-\eta_c}{2(1-\eta_c)}\cosh^2(\frac{x_{L^{opt}}}{2})-1}]$$
$$-\sqrt{2}\cosh(\frac{x_{L^{opt}}}{2})\sqrt{\cosh(x_{L^{opt}}) + \frac{3\eta_c-2}{2-\eta_c}} + \sinh(x_{L^{opt}}) = 0. \tag{4.1.12}$$

Since analytical solution of this equation is not possible, we turn once again the two cases either find perturbative solution for η_c close to the limiting value of zero (reservoirs of approximately equal temperature) and the numerical solution for different values of carnot efficiency.

4.1.1 Perturbative solution of optimized efficiency

When the temperatures of the left and the right leads are close to each other η_c becomes very small, hence we suggest that $x_{L^{opt}}$ to be expressed as series expansion in power of η_c. That is

$$x_{L^{opt}} = a_0 + a_1\eta_c + a_2\eta_c^2 + \vartheta\eta_c^3, \tag{4.1.13}$$

substitute this equation in to Eq.(4.1.12) and expanding the resulting equation in power of η_c, we get the coefficient of a_0, a_1 and a_2 by solving order by order in power of η_c. Hence, the value of $x_{L^{opt}}$ becames

$$x_{L^{opt}} = 2.39936 - 0.29992\eta_c - 0.199946\eta_C^2 + \vartheta(\eta_c^3). \tag{4.1.14}$$

To evaluate the corresponding value fore $x_{R^{opt}}$ we subestitute Eq.(4.1.14) in to Eq.(4.1.8) and taylor expand it to get

$$x_{R^{opt}} = 2.39936 + 0.29992\eta_c - 0.199946\eta_C^2 + \vartheta(\eta_c^3). \tag{4.1.15}$$

From the expression for efficiency that we defined in Eq.(2.2.3) we substitute the value of $x_{R^{opt}}$ and $x_{L^{opt}}$ to get the optimized efficiency when minimum efficiency is equal to zero, that is,

$$\eta_{opt} = 0.75\eta_c + 0.21875\eta_c^2 + 0.00651049\eta_c^3 + \vartheta(\eta_c^4). \tag{4.1.16}$$

Where as the corresponding value of the flux at optimaized function of our system becomes

$$I_{opt}^{(1)} = \alpha[\frac{1}{1+e^{x_L^{opt}}} - \frac{1}{1+e^{x_R^{opt}}}]. \tag{4.1.17}$$

From the way we calculate the flux, it is the rate at which an electron moves in the quantum dot per cycle. The period $\tau_{opt}^{(1)}$, taken to operate for one cycle at optimaized efficiency becomes

$$\tau_{opt}^{(1)} \propto \frac{1}{I_{opt}^{(1)}} = \frac{(e^{x_R^{opt}}+1)(e^{x_L^{opt}}+1)}{e^{x_L^{opt}} - e^{x_R^{opt}}}. \tag{4.1.18}$$

4.1.2 Numerical solution of optimized efficiency

In this subsection we solve for the value of $x_{L^{opt}}$ for different values of η_C numerically. Then we find the corresponding value of $x_{R^{opt}}$ from Eq.(4.1.8). Finally we substitute the values we get for $x_{L^{opt}}$ and $x_{R^{opt}}$ in Eq.(2.2.3) to find the optimized efficiency.

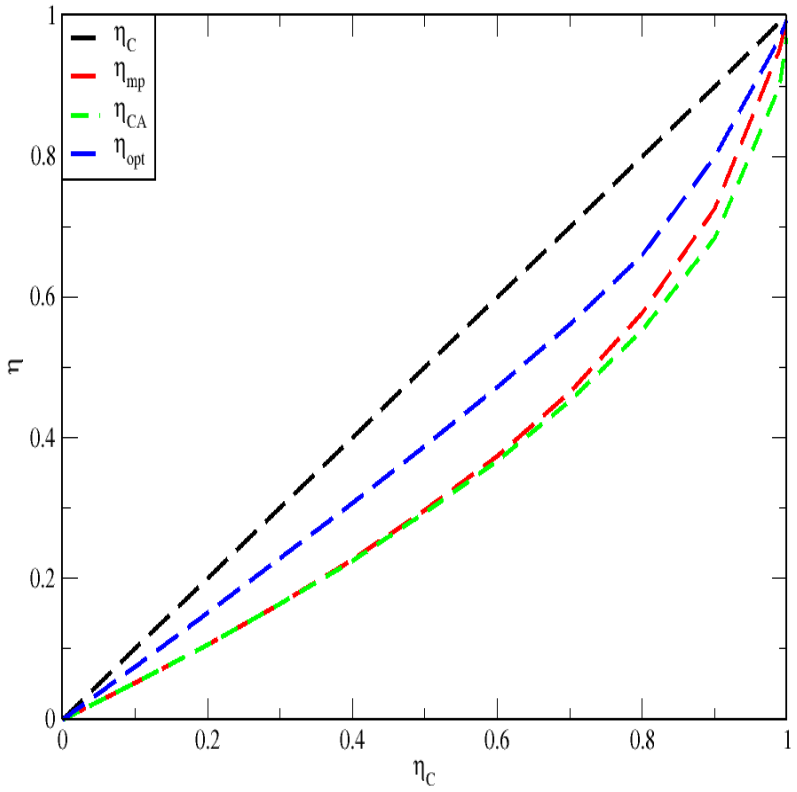

Figure 4.1: Plot of Efficiency at maximum power (red line); at optimized power efficiency when (η_{min}= 0) (blue line); at Carnot efficiency (black) and Curzon Ahlborn efficiency (green line) versus Carnot efficiency

From the Fig.(4.1) which is the numerical solution for the optimized efficiency versus Carnot efficiency. We can observe that as Carnot efficiency goes to zero the optimized efficiency goes to zero. Because when Carnot efficiency becomes very small (the temperature of the two leads approches the same) the heat flux that is getting in to the

quantum dot becames very small, as a result the optimized efficiency approches zero and as Carnot efficiency approches one (the temperature of the two leades are different) the optimized efficiency approches to one. We observed from the Fig.(4.1) the optimized efficiency increases monotonically and approaching to one. It is bounded between η_C and the efficiency at maximum power.

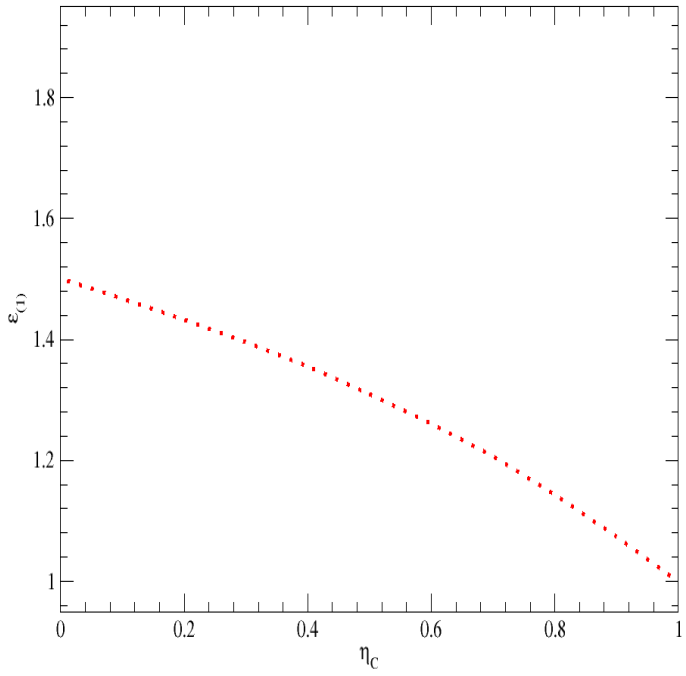

Figure 4.2: The ratio of optimized efficicency for this case of optimization criteria (when $\eta_{min} = 0$) with respect to the efficiency at maximum power versus the Carnot efficiency

From Fig.(4.2) which is the numerical solution for the ratio of optimized efficicency for this case of optimization criteria with respect to the efficiency at maximum power versus the full range of Carnot efficiency. Frome the above fig.(4.2) we can observe that as carnot efficiency goes to the maximum value (one) the ratio of optimized efficiency with respect to the effciencyiy at maximum power monotonically decrease and approaching to one .

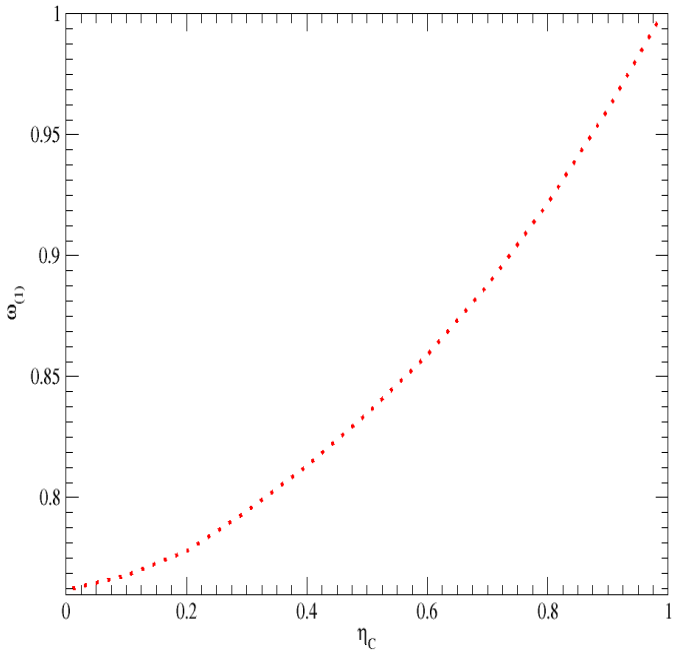

Figure 4.3: The ratio of optimized power for this cases of optimization criteria (when $\eta_{min} = 0$) with respect to the maximum power as a function of the Carnot efficiency.

From Fig.(4.3) which is the numerical solution for the ratio of optimized power for this case of optimization criteria with respect to the maximum power versus the full range of Carnot efficiency. We can observe that as carnot efficiency goes to the maximum value (one) the ratio of optimized efficiency with respect to the maximum power monotonically increase and approaching to one .Which mean that as the Carnot efficiency approching to one the maximum amount of power to be utilized.

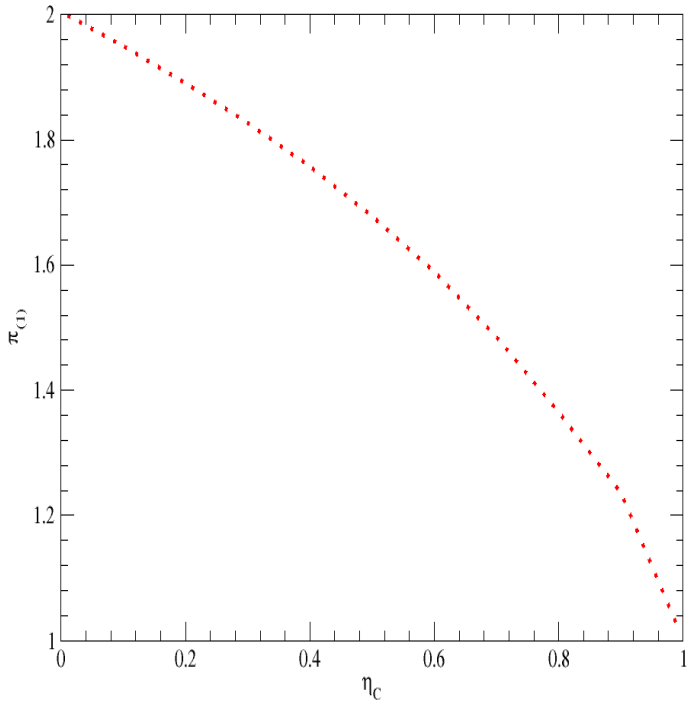

Figure 4.4: The ratio of optimized period for this cases of optimization (when $\eta_{min} = 0$) criteria with respect to the period at maximum power versus the Carnot efficiency.

From Fig.(4.4) which is the numerical solution for the ratio of optimized period for this case of optimization criteria with respect to the period at maximum power versus the Carnot efficiency. From Fig.(4.4) we can observe that as carnot efficiency goes to the maximum value one ($T_R \rightarrow$ zero), the period of performs its work decrease monotonically. However, as the Carnot efficicency goes to zero (the left lead themperature and the right lead themperature approches the same), the period of performs its work increase.

4.2 Optimized efficiency when we take minimum efficiency to be efficiency at maximum power

In this case Eq.(4.0.2) can be rewritten as

$$\dot{\Omega} = [2(1 - \frac{x_R}{x_L}(1 - \eta_c)) - \eta_{mp} - \eta_c]\alpha T_L x_L (f(x_L) - f(x_R)). \tag{4.2.1}$$

To get the optimized efficiency we first optimize the rate of objective function with respect to x_L and x_R i.e.,

$$\frac{\partial \dot{\Omega}}{\partial x_L} \mid_{{x_L}^{opt}} = f_{L^{opt}} - f_{R^{opt}} - f^2_{R^{opt}} e^{x_L^{opt}} [x_L^{opt} - 2x_R^{opt}(\frac{1 - \eta_c}{2 - \eta_{mp} - \eta_c})] = 0 \tag{4.2.2}$$

and

$$\frac{\partial \dot{\Omega}}{\partial x_R} \mid_{{x_R}^{opt}} = f_{L^{opt}} - f_{R^{opt}} + f^2_{R^{opt}} e^{x_R^{opt}} [x_L^{opt}(\frac{2 - \eta_{mp} - \eta_c}{2\eta_c - 2}) - x_R^{opt}] = 0 \tag{4.2.3}$$

Note that in the above expression $f_{L^{opt}}$ and $f_{R^{opt}}$ are the fermi distributions at optimized efficiency. Subtracting Eq.(4.2.3) from Eq.(4.2.2) we find the relationship between x_L^{opt} and x_R^{opt} as

$$\cosh(\frac{x_{R^{opt}}}{2}) = \sqrt{\frac{2 - \eta_{mp} - \eta_c}{2\eta_c - 2}} \cosh(\frac{x_{L^{opt}}}{2}) \tag{4.2.4}$$

From the identity of the hyperbolic function we know that

$$\cosh^2(\frac{x_{R^{opt}}}{2}) - \sinh^2(\frac{x_{R^{opt}}}{2}) = 1 \tag{4.2.5}$$

Substituting Eq.(4.2.4) into Eq.(4,2.5) we get

$$\sinh(\frac{x_{R^{opt}}}{2}) = \sqrt{\frac{2 - \eta_{mp} - \eta_c}{2\eta_c - 2} \cosh^2(\frac{x_{L^{opt}}}{2}) - 1} \tag{4.2.6}$$

Adding Eq.(4.2.4) and Eq.(4.2.6) and using the definition of hyperbolic function for $\cosh(\frac{x_{R^{opt}}}{2})$ and $\sinh(\frac{x_{R^{opt}}}{2})$ we get

$$e^{\frac{x_{R^{opt}}}{2}} = \sqrt{\frac{2 - \eta_{mp} - \eta_c}{2\eta_c - 2}} \cosh(\frac{x_{L^{opt}}}{2}) + \sqrt{\frac{2 - \eta_{mp} - \eta_c}{2\eta_c - 2} \cosh^2(\frac{x_{L^{opt}}}{2}) - 1} \tag{4.2.7}$$

Taking the natural Logarithm of both sides of the above equation the expression for $x_{R^{opt}}$ becames

$$x_{R^{opt}} = 2\ln[\sqrt{\frac{2-\eta_{mp}-\eta_c}{2\eta_c-2}}\cosh(\frac{x_{L^{opt}}}{2}) + \sqrt{\frac{2-\eta_{mp}-\eta_c}{2\eta_c-2}\cosh^2(\frac{x_{L^{opt}}}{2})-1}]. \quad (4.2.8)$$

After rearranging the terms in Eq.(4.2.2.) we have

$$x_{L^{opt}} - x_{R^{opt}}[\frac{2-2\eta_c}{2-\eta_{mp}-\eta_c}] + \frac{f_{R^{opt}}}{f^2_{L^{opt}}e^{x_{L0pt}}}^{-}\frac{1}{f_{L^{opt}}e^{x_{L^{opt}}}} = 0. \quad (4.2.9)$$

On the other hand

$$\frac{1}{f_{L^{opt}}e^{x_{L^{opt}}}} = 1+\cosh(x_{L^{opt}}) - \sqrt{\cosh^2(x_{L^{opt}})-1} \quad (4.2.10)$$

$$\frac{f_{R^{opt}}}{f^2_{L^{opt}}e^{x_{L0pt}}} = 2\cosh^2(\frac{x_{L^{opt}}}{2}) - 2\cosh(\frac{x_{L^{opt}}}{2})\sqrt{\cosh^2(\frac{x_{L^{opt}}}{2}) - \frac{2(1-\eta_c)}{2-\eta_{mp}-\eta_c}} \quad (4.2.11)$$

Substituting Eq.(4.2.11), Eq.(4.2.10) and Eq.(4.2.8) in to Eq.(4.2.9) we get

$$x_{L^{opt}} + \frac{4(\eta_c-1)}{2-\eta_{mp}-\eta_c}\ln[\sqrt{\frac{2-\eta_{mp}-\eta_c}{2(1-\eta_c)}\cosh(\frac{x_{L^{opt}}}{2})} + \sqrt{\frac{2-\eta_{mp}-\eta_c}{2(1-\eta_c)}\cosh^2(\frac{x_{L^{opt}}}{2})-1}]$$
$$-\sqrt{2}\cosh(\frac{x_{L^{opt}}}{2})\sqrt{\cosh(x_{L^{opt}}) + \frac{3\eta_c-\eta_{mp}-2}{2-\eta_{mp}-\eta_c}} + \sinh(x_{L^{opt}}) = 0 \quad (4.2.12)$$

Since analytical solution of this equation is not possible, we turn once again the two cases either find perturbative solution for η_c close to the limiting value of zero (reservoirs of approximately equal temperature) and the numerical solution for different value of carnot efficency.

4.2.1 Perturbative solution of optimized efficiency

When T_L and T_R close to each other η_c becomes very small, hence we suggest that $x_{L^{opt}}$ to be expressed as series expansion in power of η_c. That is

$$x_{L^{opt}} = a_0 + a_1\eta_c + a_2\eta_c^2 + \vartheta\eta_c^3 \quad (4.2.13)$$

Substitute this equation in to Eq.(4.2.12) and expanding the resulting equation in power of η_c, we get the coefficient of a_0, a_1 and a_2 by solving order by order in power of η_c. Hence, the value of $x_{L^{opt}}$ becames

$$x_{L^{opt}} = 2.39936 - 0.14996\eta_c - 0.0874768\eta_C^2 + \vartheta(\eta_c^3) \tag{4.2.14}$$

To evaluate the corresponding value for $x_{R^{opt}}$ we subestitute Eq.(4.2.14) in to Eq.(4.2.8) and taylor expand it and get $x_{R^{opt}}$.

$$x_{R^{opt}} = 2.39936 + 0.14996\eta_c - 0.0874768\eta_C^2 + \vartheta(\eta_c^30 \tag{4.2.15}$$

From the expression for efficiency that we definned in Eq.(2.3.3) we subestitute the value of $x_{R^{opt}}$ and $x_{L^{opt}}$ to get the optimized efficiency when minimum efficiency is equal maximum power efficiency that is,

$$\eta_{opt} = 0.875\eta_c + 0.03900624\eta_c^2 + 0.0225361\eta_c^3 + \vartheta(\eta_c^4). \tag{4.2.16}$$

Where as the corresponding value of the flux at optimaized function of our system becomes

$$I_{opt}^{(2)} = \alpha[\frac{1}{1+e^{x_L^{opt}}} - \frac{1}{1+e^{x_R^{opt}}}]. \tag{4.2.17}$$

From the way we calculate the flux, it is the rate at which an electron moves in the quantum dot per cycle. The period $\tau_{opt}^{(2)}$, taken to operate for one cycle at optimaized efficiency becomes

$$\tau_{opt}^{(2)} = \frac{1}{I_{opt}^{(2)}} = \frac{(e^{x_R^{opt}}+1)(e^{x_L^{opt}}+1)}{\alpha(e^{x_L^{opt}} - e^{x_R^{opt}})}. \tag{4.2.18}$$

4.2.2 Numerical solution of optimized efficiency

In this subsection we solve for the value of $x_{L^{opt}}$ for different values of η_C numerically. Then we find the corresponding value of $x_{R^{opt}}$ from Eq.(4.2.8). Finally we substitute the values we get for $x_{L^{opt}}$ and $x_{R^{opt}}$ in Eq.(2.2.3) to find the optimized efficiency.

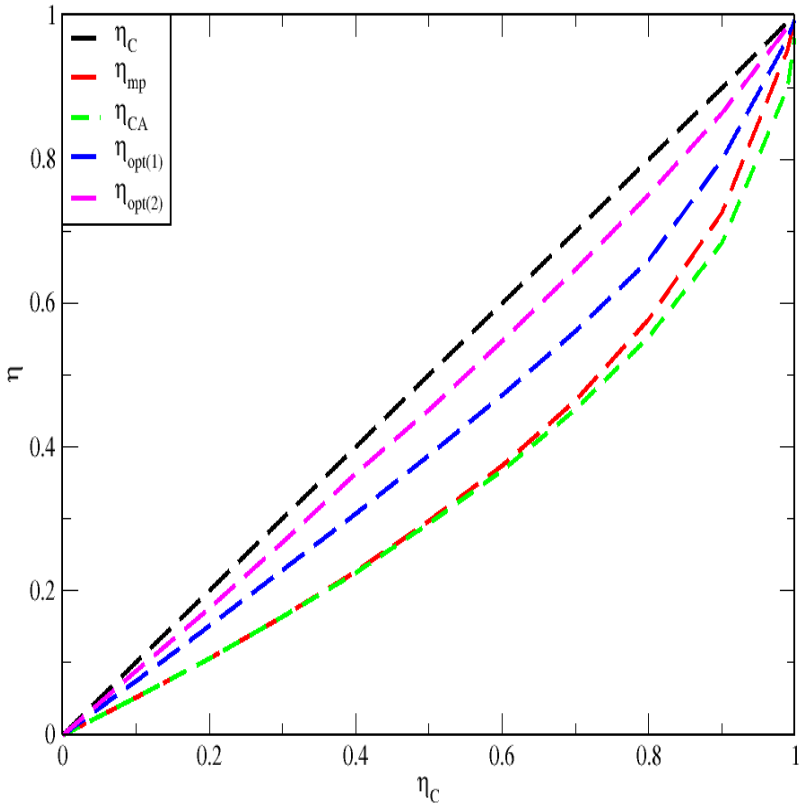

Figure 4.5: Plot of Efficiency at maximum power (red line); at optimized power efficiency when (η_{min}= η_{mp}) (magenta line); at optimized power efficiency when (η_{min}= 0) (blue); at Carnot efficiency (black) and Curzon Ahlborn efficiency (green line) versus Carnot efficiency

From the Fig.(4.5) we can observe that as Carnot efficiency goes to zero the optimized efficiency goes to zero. This is because when Carnot efficiency becames very small(i.e. as the temperature of the two leads approches the same) the heat flux that is getting in to the quantum dot becames verry small, hence the optimized efficiency approches zero

where as Carnot efficiency approches one (i.e. as the temperature of the two leades are different) the optimized efficiency approches to one.

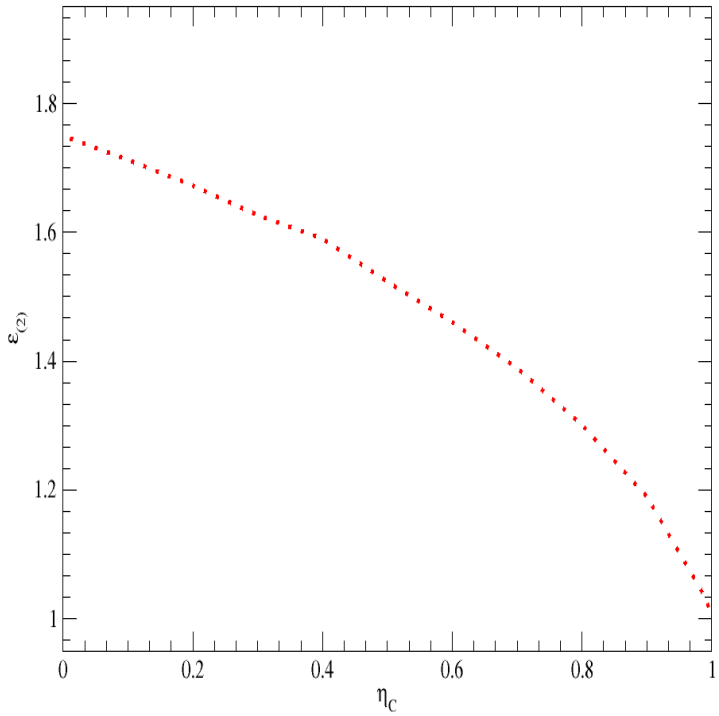

Figure 4.6: The ratio of optimized efficicency for this optimization criteria (when $\eta_{min} = \eta_{mp}$) with respect to the efficiency at maximum power versus the Carnot efficiency

From Fig.(4.6) which is the numerical solution for the ratio of optimized efficicency for this case of optimization criteria with respect to the efficiency at maximum power versus the full range of Carnot efficiency. We can observe that as carnot efficiency goes to the maximum value one ($T_R \rightarrow$ zero) the ratio of optimized efficiency with respect to the effciencyiy at maximum power monotonically decrease and approaching to one .

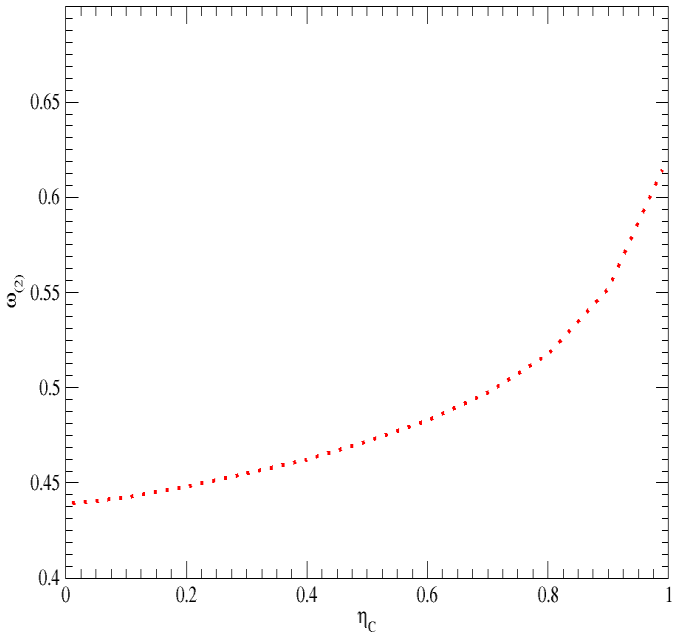

Figure 4.7: The ratio of optimized power for this cases of optimization criteria $\eta_{min} = \eta_{mp}$) with respect to the maximum power as a function of the Carnot efficiency.

From Fig.(4.7) which is the numerical solution for the ratio of optimized power for this case of optimization criteria with respect to the maximum power versus the full range of Carnot efficiency. We can observe that as carnot efficiency goes to the maximum value ($T_R \rightarrow$ zero) one the ratio of optimized efficiency with respect to the maximum power monotonically increase. Which mean that Carnot efficiency approching to one the maximum amount of power to be utilized.

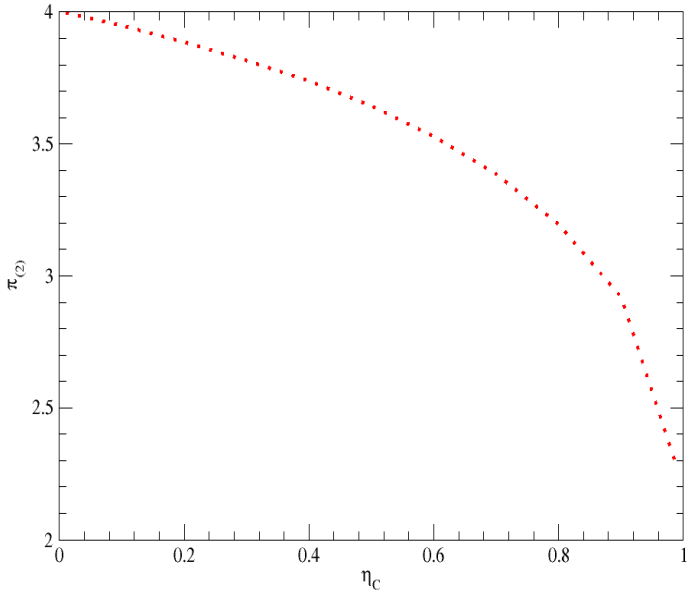

Figure 4.8: The ratio of optimized period for this cases of optimization criteria $\eta_{min} = \eta_{mp}$) with respect to the period at maximum power versus the Carnot efficiency.

From Fig.(4.8) which is the numerical solution for the ratio of optimized period for this case of optimization criteria with respect to the period at maximum power versus the Carnot efficiency. We can observe that as carnot efficiency goes to the maximum value one($T_R \rightarrow$ zero), the period of performs its work decrease monotonically. However, as the Carnot efficicency goes to zero (i.e. the left and the right lead themperature approches the same), the period of performs its task monotonically increase.

We define a figure of merit, a quantity used to characteraize the performance of a divice (heat engine) or a numerical quantity based on the characterstics of a heat engine that represents a measure of effictiveness, f_m, defined by

$$f_m = \frac{\varepsilon\omega}{\pi} \tag{4.2.19}$$

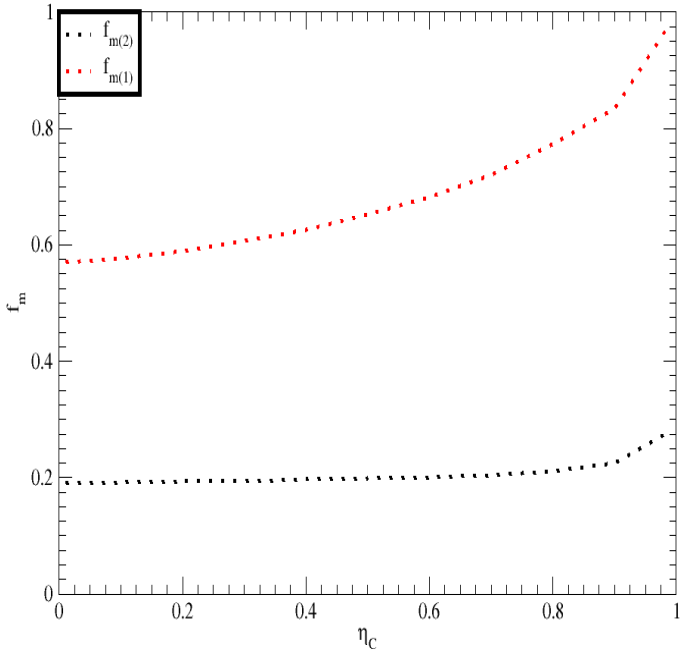

Figure 4.9: Figure of merit versus the Carnot efficiency.

Figure (4.9) plots the figure of merit, $f_m(1)$ and $f_m(2)$, versus η_C . We observe from the Fig.(4.9) Carnot efficency increase both figure of merit increase. Comparing the above plots one clearly sees that the first optimization has better performance over the second for the whole range of Carnot efficiency. We observe that the performance of the first optimization is three times better than the second one.

Chapter 5

Summary and Conclusion

In this work, we considered a stochastically driven single level quantum dot embedded between two metallic leads at different temperatures which work as a heat engine. The simplicity of the model enabled us to perform two ways of optimization criteria to find their corresponding optimized efficiencies, powers, periods and figure of merits as a function of Carnot efficiency.

After we calculated the efficiency at maximum power for our model which work as a heat engine, we introduced an objective function based on the proposal of Hernandez et.al.[7]. Using optimization principle we optimized the objective function with respect to the right lead electron scaled energy and the left lead electron scaled energy, 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. After this we compared efficiencies: Carnot efficiency, Curzon-Ahlborn effciency, efficiency at maximum power, and optimized efficiency. Carnot efficiency which is the maximum efficiency but it takes infinite 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 [6] 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 graph. Finally, we have optimized efficiency which lies between efficiency at maximum power and Carnot efficiency which tells us it is the best.

In general, we believe that our work has, for the first time, found an optimized efficiency which is between the efficiency at maximum power (and also Curzon - Ahlborn [6]) and maximum efficiency (Carnot efficiency) analytically, when the temperatures of the heat reservoirs are nearly equal, numerically we obtained an optimized efficiencies that lies between the two efficiencies for the model we considered. And also the numerical solution illustrates that efficiencywise the second optimization is more advantageous than the first optimization over all range of η_c . However, while this advantage is significant for smaller η_c it shrinks to the same value when η_c goes to one. Finally we conclude that the first optimization(takes as minimum efficiency equal to zero) is advantageous than the second case of optimization (takes as minimum efficiency the efficeney at maximum power) as well as the first case of optimization utilizes a large amount of maximum power at small value of η_c and performs even better as η_c goes to one. The performance of the first optimization better than three times the second one.

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Declaration

This thesis is my original work, has not been presented for a degree in any other University and that all the sources of material used for the thesis have been dully acknowledged.

Name: Yigermal Bassie Yassabie

Signature:– – – – – – – – – – – –

Place and time of submission: Addis Ababa University, June 2012

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

Name: Dr.Mulugeta Bekele

Signature:– – – – – – – – – ––