THERMODYNAMIC PROPERTIES OF TWO QUANTUM DOTS CONNECTED IN PARALLEL

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Abstract

In this thesis we take single level two quantum dots connected in parallel between two metalic leads at different temperature and chemical potential which works as a heat engine. After calculating the current for the thermoelectric engine we evaluate other thermodynamic quantities such as heat flux, power and efficiency. We also study how our model behaves as a function of a quantity (Δ) that characterizes the energy level difference between the two dots

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Chapter 1

Introduction

A heat engine typically uses energy provided in the form of heat to do work and then exhausts the heat which can not be used to do work. Thermodynamics is the study of the relationships between heat and work. The First and Second Laws of thermodynamics constrain the operation of a heat engine. The First Law is the application of conservation of energy in a system, and the Second Law sets limits on the possible efficiency of the machine and determines the direction of energy flow. In order to illustrate how a heat engine works, we consider gas in a container whose volume is allowed to expand(or contract). We assume the working substance to be a monoatomic ideal gas.

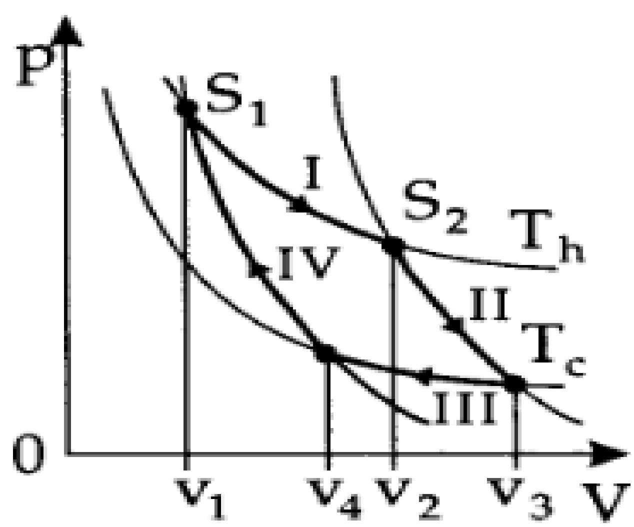

Figure 1.1: P-V diagram of heat engine undergoing Carnot cycle

The Carnot cycle performs as an engine, converting part of the heat transfered to the gas during the process in to useful work. The Carnot process is performed in four successive reversible steps, which we illustrate in a P-V diagram as shown in Fig.1.1.

Step 1: Isothermal expanision from volume V_1 to V_2 at constant temprature T_h. For the isothermal process, the volumes(V_1 and V_2) and their corresponding pressures (P_1 and P_2) are related by:

$$\frac{V_2}{V_1} = \frac{P_1}{P_2}. \tag{1.0.1}$$

The internal energy of an ideal gas does not change at constant temprature. Consequently it holds that

$$\Delta U_1 = \Delta Q_1 - \Delta W_1 = 0 \tag{1.0.2}$$

where ΔU_1, ΔW_1, ΔQ_1 are the internal energy, work done by the system, and heat added to the gas respectively. From this we can calculate ΔQ_1, so that

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

Where N is number of molecule in a container and k_B is Boltzmann constant.

This is the amount of heat that the system absorbed from the heat bath from the first step. Since $V_2 > V_1, \Delta Q_1 > 0$; so that the amount of heat ΔQ_1 is added to the gas from the heat bath.

Step 2: Adiabatic expanision of the isolated working material from V_2 to V_3. Here the temprature changes from $T_h$to T_c. The indices h and c denotes hot and cold, i.e., $T_h > T_c$:

$$\frac{V_3}{V_2} = (\frac{T_h}{T_c})^{3/2} \tag{1.0.4}$$

Since $\Delta Q_2 = 0$ (for adiabatic process) the work ΔW_2 performed by the expanision is taken from the internal energy and hence is given by

$$-\Delta W_2 = \Delta U_2 = C_v(T_c - T_h) \tag{1.0.5}$$

For a monoatomic ideal gas , $C_v = \frac{3Nk_B}{2}$, i.e., C_v is a constant independent of temprature and volume.

Step 3: We now compress the system isothermally from V_3 to V_4 at the (constant) lower temprature T_c. Analogous to step 1 we have

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

The work performed during the compression is, because $\Delta U_3 = 0$ at $T =$ constant temperature, submitted to the heat bath in form of heat.

$$\Delta U_3 = \Delta Q_3 - \Delta W_3 = 0 \tag{1.0.7}$$

$$\Delta Q_3 = \Delta W_3 = N k_B T_c \ln \frac{V_4}{V_3} \tag{1.0.8}$$

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 initial state via an adiabatic compression from V_4 to V_1. The temprature increases from T_c to T_h such that

$$\frac{V_1}{V_4} = (\frac{T_c}{T_h})^{3/2}. \tag{1.0.9}$$

Since $\Delta Q_4 = 0$ it follows that

$$-\Delta W_4 = \Delta U_4 = C_v(T_h - T_c) \tag{1.0.10}$$

Let us first check the total energy balance of the process in one cycle is

$$\Delta U_{total} = \Delta Q_1 - \Delta W_1 - \Delta W_2 + \Delta Q_3 - \Delta W_3 - \Delta W_4 \tag{1.0.11}$$

If we insert Equ. (1.0.3) (1.0.5) (1.0.8) (1.0.10), 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 simillarly $\Delta Q_3 - \Delta W_3 = 0$, and furthermore $\Delta W_2 = -\Delta W_4$. In addition, we have the following equations for the amount of heat exchanged with the heat bath:

$$\Delta Q_1 = N k_B T_h \ln \frac{V_2}{V_1} \tag{1.0.12}$$

$$\Delta Q_3 = N k_B T_c \ln \frac{V_4}{V_3}$$

On the other hand from Eq. (1.0.4) (1.0.9),we have

$$\frac{V_3}{V_2} = \frac{V_4}{V_1} \tag{1.0.13}$$

$$\frac{V_2}{V_1} = (\frac{V_4}{V_3})^{-1}$$

Then, however, for ΔQ_1 and ΔQ_3 we have, according to Equation (1.0.12) that

$$\frac{\Delta Q_1}{T_h} + \frac{\Delta Q_3}{T_c} = 0 \tag{1.0.14}$$

This equation is of great importance, for it valid not only for our special Carnot process, but for any reversible cyclic process.

The Carnot process effectivelly performs a work ΔW:

$$\begin{aligned} \Delta W &= \Delta W_1 + \Delta W_2 + \Delta W_3 + \Delta W_4 \\ &= N k_B T_h \ln \frac{V_2}{V_1} + N k_B T_c \ln \frac{V_4}{V_3} \end{aligned}$$

and using Eq. (1.0.13)

$$\begin{aligned} \Delta W &= N k_B (T_h - T_c) \ln \frac{V_2}{V_1} \\ &= (\Delta Q_1 + \Delta Q_3) \end{aligned}$$

Since $T_h > T_c$ and $V_2 > V_1$, this is a positive quantity. Hence, ΔW is work performed by the gas. obviously , a Carnot engine is an engine which transforms heat in to work. The work performed by the engine increases with the temprature difference $T_h - T_c$ and with the compression ratio $\frac{V_2}{V_1}$. We now want to calculate the efficiency of this engine.
Efficiency is the ratio of the output energy to the total heat input (or input energy),

$$\eta_c = \frac{\Delta W}{\Delta Q_1} \tag{1.0.15}$$

Substitution of Δw and ΔQ_1 by their values given above will yield:

$$\eta_c = 1 - \frac{T_c}{T_h} \tag{1.0.16}$$

A reversible operation or reversible cycle is a process that can be "revesed" by means of infinitesmal change in some property of the system with out loss or dissipation of energy. Since it would take an infinite amount of time for the reversible process to finish, the power which the engine performs is zero($\dot{W} = W/t = 0, t \longrightarrow \infty$).

Thermoelectricity refers to a class of phenomena in which a temperature difference creates an electric potential or an electric potential creates a temperature difference. In modern technical usage, the term refers collectively to the Seebeck effect, Peltier effect, and the Thomson effect [1]. Various metals and semiconductors are generally employed in these applications. One of the most commonly used material in such applications is Bismuth telluride (Bi_2Te_3).

The discovery of thermoelectricity date back to Thomas John Seebeck(1770-1831). In 1821, he discovered that a compass needle deflected when placed in the vicinity of a closed loop formed from two dissimilar metal conductors if the junctions were maintained at different tempratures. The magnitude of the deflection was proportional to the temprature difference and depend on the type of conducting material.
Later Jean Peltier described thermal effects at the junctions of dissimilar conductors when an electrical current flows between the materials in 1834.
In 1851, William Thomson(later Lord Kelvin) observed the cooling or heating of a homogeneous conductor resulting from the flow of an electrical current in the presence of a temprature gradient. This is known as the Thomson effect and is defined as the rate of heat generated or absorbed in a single current carrying conductor subjucted to a temprature gradient.

The field of thermoelectricity went through a revival in the early 1990s due to the discovery of new thermoelectric materials with significantly higher thermodynamic yields [2]. Of particular interest are the developments in the context of nanostructured materials [3]. For example, thermoelectric experiments have been reported on silicon nanowires [4], individual carbon nanotubes [5] and molecular junctions [6]. Furthermore , it has been reported that Carnot efficiency can be reached for electron transport between two leads at different temperatures and chemical potentials, by connecting them through a channel sharply tuned at the energy for which the electron density is the same in both leads [7,8]. A double-barrier resonant tunneling structure has been proposed as a possible technological implementation [9].

An equation for the efficiency of semi-ideal heat engine operating at maximum power out put in which heat transfer is irreversible, which is the Curzon-Ahlborn efficiency[10].

$$\eta_{CA} = 1 - \sqrt{\frac{T_c}{T_h}} = 1 - \sqrt{1-\eta_c} \approx \frac{\eta_c}{2} + \frac{\eta_c^2}{8} + \frac{6\eta_c^3}{96} + ... \tag{1.0.17}$$

Recently, it has been that the Curzon-Ahlborn efficiency is an exact consquence of linear irreversible thermodynamics when operating under conditions of strong coupling between the heat flux and the work. The value of $\frac{1}{2}$ for the linear coefficient in eq.(1.0.17) is therfore universal for such systems.

The above results agree, as they should [11], to linear order η_c. More surprisingly, the coefficient of the quadratic term is also identical.

In a previous work considered a model tiny heat engine (with a single level quantum dots) in contact with hot and cold heat reservoirs proposed by M.Esposito et .al [12]. This proposed model is composed of a quantum dot embeded between two metalic leads at different temperatures and chemical potentials. They studied how the device operates and determined the efficiency at maximum power and compared their value with that of the Curzon-Alhborn efficiency [10]. But in this work, we will consider a model tiny heat engine (single level two quantum dots) in contact with hot and cold reservoirs. All other operations are the same as the previous work of heat engine with a single level .

The rest of this work is organized as follows . In Chapter 2, we derive the thermodynamic quantities such as: current, heat flux, power, and efficiency for two single-level quantum dot connected in parallel between two heat reservoirs. In Chapter 3 we evaluate and explore the behaviors of heat flux, power and efficiency as a function of energy parameter a scaled $\frac{\Delta}{\epsilon}$ characterizing the energy difference between the two levels. In Chapter 4, we evaluate the efficiency at maximum power by using a purturbative solution and numerical solution and the result that we get for the efficiency at maximum power lies between the Carnot efficiency and Curzon-Ahlborn efficiency.

Finally, Chapter 5 deals with summary and conclusion.

Chapter 2

Thermoelectric efficiency in two quantum dots connected in parallel

Quantum dots are semicoductor nanocrystals that are so small. They are practically considered dimensionless. They are tiny nanocrystals that glow (to produce light and/or heat with out smoke or flames) when stimulated by an external source such as Ultraviolet (UV) light. How many atoms are included in the quantum dots determines their size and the size of the quantum dot determines the colour of light emmited.

Quantum dots are more closely related to an atom than a bulk material because of their discrete, quantized energy level. Band gaps, depends on the relationship between the size of the crystal and the exciton Bohr radius. In the strong confinement regime the band gapis smaller where the size of the quantum dots is smaller than the exciton Bohr radius as the energy levels split up. Due to the energy level split up the emission energy becomes increases (the sum of the energy level in the smaller band gaps in the strong confinment regime is larger than the energy levels in the band gaps of the original levels in the weak confinment regime) and the emission at various wavelength. The quantum dot energy level split up to the degree that the energy spectrum is almost continuous thus the quantum dot emits white light. The smaller quantum dots have higher energy, smaller wavelength and go toward blue colour and the larger quantum dots have smaller energy, higher wavelength and go toward red colour shown Fig.2.1. Quantum dots can be synthesized to be essentially any size, and therefore, produce essentially any wave length

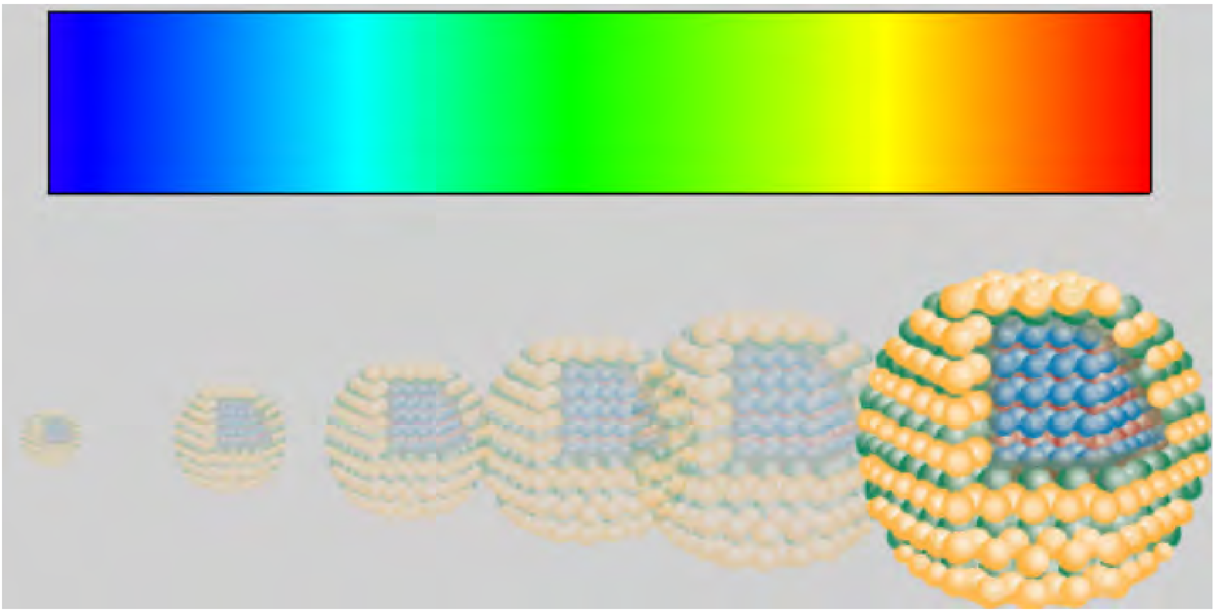

Figure 2.1: The size of the quantum dot corresponding with colours

of light. It can be made from a range of materials (2nm-10nm in diameter), currently the most commonly used materials include zinc sulphide, lead sulfide, cadmium selenide and Indium Phosphide. Many of the promissing applications for quntum dots will be used with in the human body [13].

In the rest of this Chapter we take two quantum dots that work as thermoelectric engine and use stochastic thermodynamic method to find quantities such as current, heat flux, power, efficiency and entropy.

2.1 Derivation of thermoelectic efficiency in a two quantum dot with corresponding energy level

2.1.1 The model and derivation of the thermodynamic quantities

Two quantum dots are connected in parallel to two (hot and cold) heat reserviors of tempratures T_r and T_l, respectively as shown in Fig.2.2. The contacts to which the quantum dots are connected have chemical potentials μ_r and μ_l as shown in the same figure.

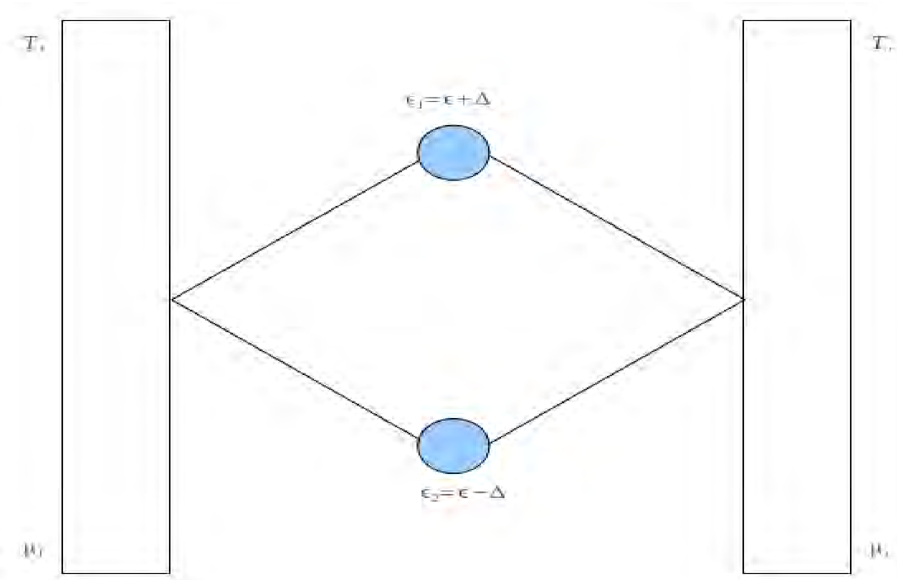

Figure 2.2: Sketch of nano thermoelectric engine consist of a two quantum dot embeded between two leads at different temprature and chemical potentials. We choose by convention $T_l < T_r$.

. Due to their size variation, the quantum dots have different single energy levels associated with each of them. Accordingly, we consider the single energy level of the first quantum dot ϵ_1 to be $\epsilon + \Delta$ while that of the second quantum dot ϵ_2 to be $\epsilon - \Delta$. The temprature and chemical potential difference between the two contacts generate current through the two quantum dots through electron hopping to (or from) the leads to the quantum dot which is either empty or filled.

We assume that the electrons thermalize instantaneously to temperature of the leads $T_r(T_l)$ upon tunnelling to the reservoirs. In order to describe the basic mechanism to produce heat and work, we assume that the energy of the level is varied in time. Upon varying the energy of the level, a certain amount of (positive or negative) energy flows into the system in the form of heat and work. If the level occupied by an electron while it is lowered (raised), power is extracted from (injected into) the system, $W < 0 (W > 0)$. If the level remains empty while its energy is changed, neither power nor heat flux are produced. When the empty (filled) level at energy $\epsilon + \Delta$ and $\epsilon - \Delta$ is filled (emptied) by

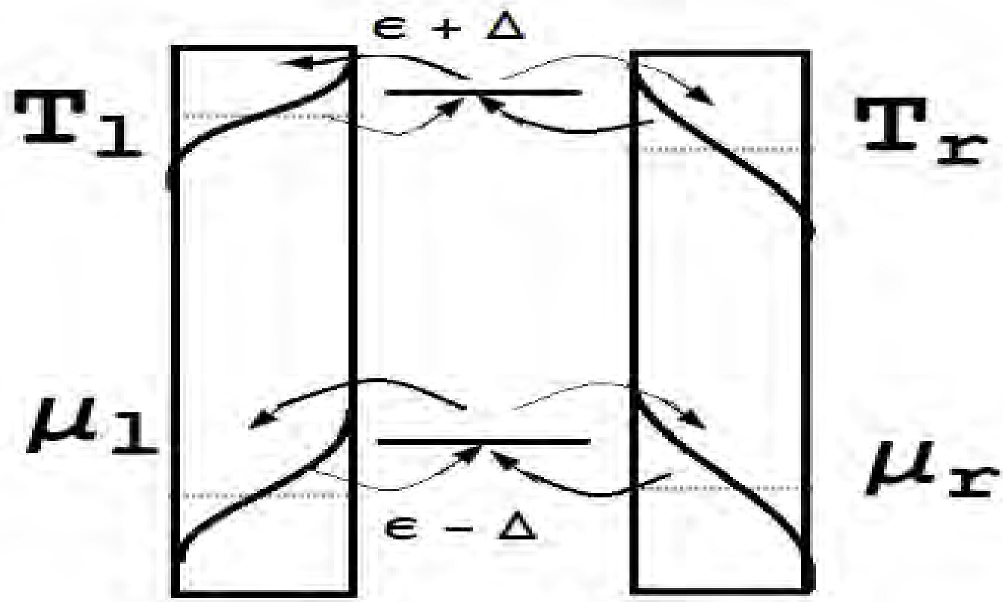

Figure 2.3: Sketch of nano thermoelectric engine consist of a two quantum dot embeded between two leads at different temprature and chemical potentials. We choose by convention $T_l < T_r$.

an electron, an amount of heat flux $Qr(Ql)$ enters the system.

We now turn to the mathematical analaysis of the thermoelectric engine represented in fig.2.2. A two quantum dot, with orbital energy $\epsilon + \Delta$ and $\epsilon - \Delta$, exchanges electrons with a cold left lead, temprature T_l and chemical potential μ_l, with a hot right lead, temprature T_r and chemical potential μ_r. The quantum dot is either empty(state 1) or filled(state 2) for the first quantum dot and the second quantum dot either empty(state 3) or filled(state 4).

The crucial variables of the problem are the scaled energy barriers with($k_B = 1$). The scaled energy barriers of the first quantum dot is

$$x_v = (\epsilon + \Delta - \mu_v)/T_v \tag{2.1.1}$$

where, $v = l, r$

the scaled energy barriers of the second quantum dot is

$$y_v = (\epsilon - \Delta - \mu_v)/T_v \tag{2.1.2}$$

where, $v = l, r$

The exchange of electrons with the leads in the first quantum dot is described by the following quantum master equation [14-16]:

$$\begin{pmatrix} \dot{p}_1(t) \\ \dot{p}_2(t) \end{pmatrix} = \begin{pmatrix} -W_{21} & W_{12} \\ W_{21} & -W_{12} \end{pmatrix} \begin{pmatrix} p_1(t) \\ p_2(t) \end{pmatrix} \tag{2.1.3}$$

where $\dot{p}_{1(2)}(t)$ is the rate of occupational probablity when the first quantum dot is empty(filled) at a time t and W_{ij} is the transitional rate from state j to i. Here i and j take the value 1 and 2.

The exchange of electrons with the leads in the second quantum dot is described by the following quantum master equation [14-16]:

$$\begin{pmatrix} \dot{p}_3(t) \\ \dot{p}_4(t) \end{pmatrix} = \begin{pmatrix} -W_{43} & W_{34} \\ W_{43} & -W_{34} \end{pmatrix} \begin{pmatrix} p_3(t) \\ p_4(t) \end{pmatrix} \tag{2.1.4}$$

$\dot{p}_{3(4)}(t)$ is the rate of occupational probability when the second quantum dot is empty (filled) at a time t and W_{ks} is the transitional rate from state s to k. Here k and s takes the value 3 and 4. The transitional rate in the first quantum dot is given by

$$W_{12} = \sum_{v=l,r} W_{12}^{(v)} = \sum_{v=l,r} a_v(1 - f_v) \tag{2.1.5}$$

$$W_{21} = \sum_{v=l,r} W_{21}^{(v)} = \sum_{v=l,r} a_v f_v \tag{2.1.6}$$

Where a_v is the Einstein coefficient which is independent of the quantum dot energy known as the wide-band approximation. While f_v is the Fermi distribution which is given by

$$f_v = [exp(x_v) + 1]^{-1} \tag{2.1.7}$$

Where $v = l, r$

The transitional rate of the second quantum dot is given by

$$W_{34} = \sum_{v=l,r} W_{34}^{(v)} = \sum_{v=l,r} b_v(1 - g_v) \tag{2.1.8}$$

$$W_{43} = \sum_{v=l,r} W_{43}^{(v)} = \sum_{v=l,r} b_v g_v \tag{2.1.9}$$

Where b_v is the Einstein coefficient which is indepent of the dot energies known as the wide-band approximation. While g_v is the Fermi distribution which is given by

$$g_v = [exp(y_v) + 1]^{-1}, v = l, r \tag{2.1.10}$$

We are interested in the property of the device at the steady state. The steady state distribution for the first quantum dot occupation and the second quantum dot occupation is respectively

$$\dot{p}_1(t) = \dot{p}_2(t) = 0$$

$$\dot{p}_3(t) = \dot{p}_4(t) = 0 \tag{2.1.11}$$

Then from equation (2.1.3) and (2.1.4)

$$W_{21}p_1^{ss} = W_{12}p_2^{ss} \tag{2.1.12}$$

$$W_{43}p_3^{ss} = W_{34}p_4^{ss} \tag{2.1.13}$$

Where $p_{1(2)}^{ss}$ are the steady state occupational probability for empty(filled) state of the first quantum dot and

$p_{3(4)}^{ss}$ are the steady state occupational probability for empty(filled) state of the second quantum dot.

The resulting steady state electron current entering the first quantum dot from lead v is given by

$$I_v = W_{21}^{(v)}p_1^{ss} - W_{12}^{(v)}p_2^{ss}, v = l, r \tag{2.1.14}$$

Hence the probability current I_r and I_l entering from the right and the left lead to the first quantum dot are respectively given by

$$\begin{aligned} I_r &= W_{21}^{(r)}p_1^{ss} - W_{12}^{(r)}p_2^{ss} \\ I_l &= W_{21}^{(l)}p_1^{ss} - W_{12}^{(l)}p_2^{ss} \end{aligned} \tag{2.1.15}$$

Substituting eq. (2.1.5) and (2.1.6) from eq. (2.1.12) and rearranging we can get $I_r = -I_l$.

The resulting steady state electron current entering the second quantum dot from lead v is given by

$$J_v = W_{43}^{(v)}p_3^{ss} - W_{34}^{(v)}p_4^{ss} \tag{2.1.16}$$

Hence the probability current J_r and J_l entering from the right and the left lead to the second quantum dot are respectively given by

$$\begin{aligned} J_r &= W_{43}^{(r)}p_3^{ss} - W_{34}^{(r)}p_4^{ss} \\ J_l &= W_{43}^{(l)}p_3^{ss} - W_{34}^{(l)}p_4^{ss} \end{aligned} \tag{2.1.17}$$

Substituting eq. (1.2.8) and (1.2.9) into eq. (1.2.13) and rearranging them we can get $J_r = -J_l$. and also

$$\begin{aligned} W_{12} + W_{21} &= a_r + a_l \\ W_{34} + W_{43} &= b_r + b_l \end{aligned} \tag{2.1.18}$$

But the wide-band approximation is independent of the dot energy, so $a_r = b_r$ and $a_l = b_l$. Now let us see how our device (the quantum dot) works as a heat engine. The quantum dot gets a steady state heat flux $\dot{Q}_r$ from the right lead (i.e from the hot reservoirs) and extracts net power $\dot{W}$ while dissipating a steady state heat flux of $\dot{Q}_l$ to the left lead (i.e to the cold reservoir).

The steady state flux entering in to the first quantum dot from the lead v is $\dot{Q}_v'$ is defined as:

$$\dot{Q}_v' = (\epsilon + \Delta - \mu_v)I_v, v = l, r \tag{2.1.19}$$

The steady state flux entering into the second quantum dot from lead v is $\dot{Q}_r''$ is defined as

$$\dot{Q}_v'' = (\epsilon - \Delta - \mu_v)J_v, v = l, r \tag{2.1.20}$$

.

The total heat flux entering in to the quantum dot from lead v

$$\dot{Q}_v = \dot{Q}_v' + \dot{Q}_v'' \tag{2.1.21}$$

Using the normalization condition ($p_1^{ss} + p_2^{ss} = 1$) the probability current entering the first quantum dot from the right lead becomes

$$I_r = W_{21}^{(r)} - (W_{12}^{(r)} + W_{21}^{(r)})p_2^{ss} \tag{2.1.22}$$

Using the normalization condition ($p_1^{ss} = 1 - P_2^{ss}$) and substituting p_1^{ss} into equation (1.2.12) we can get

$$p_2^{ss} = \frac{(a_r f_r + a_l f_l)}{a_r + a_l} \tag{2.1.23}$$

Substituting equation (1.2.23) into equation (1.2.22) becomes

$$I_r = \alpha(f_r - f_l) \tag{2.1.24}$$

where $\alpha = \frac{(a_r a_l)}{a_r + a_l}$

Using the normalization condition ($p_3^{ss} + p_4^{ss} = 1$) the probablity current entering from the right lead becomes

$$J_r = W_{43}^{(r)}(1 - p_4^{ss}) - W_{34}^{(r)}p_4^{ss} \tag{2.1.25}$$

Insrrting ($p_3^{ss} = 1 - p_4^{ss}$) in to equation (1.2.13) becomes

$$p_4^{ss} = \frac{(b_r g_r + b_l g_l)}{b_r + b_l} \tag{2.1.26}$$

substituting equation (1.2.26) into (1.2.25) becomes

$$J_r = \gamma(g_r - g_l) \tag{2.1.27}$$

where $\gamma = \frac{(b_r b_l)}{b_r + b_l}$

But $\alpha(\gamma)$ is the Landauer formula for a single channel. These two constants are also independant of dot energy so, lets assume the two constant are equal.

The heat flux entering from right to the first quantum dot $\dot{Q}_r^{'}$ becomes

$$\dot{Q}_r^{'} = (\epsilon + \Delta - \mu_r)I_r = \alpha T_r x_r (f_r - f_l) \tag{2.1.28}$$

and for the second quantum dot

$$\dot{Q}_r^{''} = (\epsilon - \Delta - \mu_r)J_r = \alpha T_r y_r (g_r - g_l) \tag{2.1.29}$$

Total heat flux entering into a quantum dot from right lead(hot reservoir)

$$\dot{Q}_r = \dot{Q}_r^{'} + \dot{Q}_r^{''} \tag{2.1.30}$$

$$\dot{Q}_r = \alpha T_r [x_r (f_r - f_l) + y_r (g_r - g_l)] \tag{2.1.31}$$

The heat flux desipates in to the cold reservior(lead) from the second quantum dot is $\dot{Q}_l^{''}$ given by

$$\dot{Q}_l^{''} = (\epsilon - \Delta - \mu_l)J_l = -(\epsilon - \Delta - \mu_l)J_r$$

$$\dot{Q}_l^{''} = -\alpha T_l y_l (g_r - g_l) \tag{2.1.32}$$

The total heat flux dissipates in to a cold reservior(lead l) from the second quantum dot is $\dot{Q}_l$

$$\dot{Q}_l = \dot{Q}_l' + \dot{Q}_l'' \tag{2.1.33}$$

$$= -\alpha T_l[x_l(f_r - f_l) + y_l(g_r - g_l)] \tag{2.1.34}$$

The net power output by the quantum dot is the sum of total heat flux getting in to it and dissipates heat into cold reservior:

$$Power = \dot{W} = \alpha T_r[x_r(f_r - f_l) + y_r(g_r - g_l)] - \alpha T_l[x_l(f_r - f_l) + y_l(g_r - g_l)] \tag{2.1.35}$$

The efficiency of the thermoelectric engine is

$$efficiency = \frac{poweroutput}{inputheatflux} \tag{2.1.36}$$

$$\eta = \frac{\dot{W}}{\dot{Q}_r} \tag{2.1.37}$$

$$\eta = \frac{(f_r - f_l)[x_r - (1-\eta_c)x_l] + (g_r - g_l)[y_r(1-\eta_c)y_l]}{x_r(f_r - f_l) + y_r(g_r - g_l)} \tag{2.1.38}$$

2.2 The Carnot efficiency

2.2.1 Entropy

Entropy addresses these question regarding the transformation of the form of energy and tell us how much energy can be converted from one form to another, and in particular, how much energy is available for doing usefull work.

The entropy production associated with the master eq. (2.1.3) and eq. (2.1.4) is given by [17-20] in the case of the first quantum dot

$$\sigma_1 = \sum_{i,j,v} W_{ij}^{(v)} p_j^{ss} \ln \frac{W_{ij}^{(v)} p_j^{ss}}{W_{ji}^{(v)} p_i^{ss}}; \tag{2.2.1}$$

where $i, j = 1, 2$. Noting that $\ln [W_{12}^{(v)}/W_{21}^{(v)}] = x_v$, one finds, in agreement with standard irrevesible thermodynamics [21], the following expression for the entropy production:

$$\sigma_1 = F_m J_m + F_e J_e = \alpha(x_l - x_r)(f_r - f_l) \geq 0 \tag{2.2.2}$$

With thermodynamics forces for matter and energy flow, F_m and F_e, given by

$$F_m \equiv -(\frac{\mu_r}{T_r} - \frac{\mu_l}{T_l}), F_e \equiv \frac{1}{T_r} - \frac{1}{T_l} \tag{2.2.3}$$

We stress that the corresponding matter and heat flow, given by

$$J_m = -I_r, J_e = -(\epsilon + \Delta)I_r \tag{2.2.4}$$

The entropy production associated with the master eq. (1.2.3) and eq. (1.2.4) is given by [17-20] in the case of the second quantum dot

$$\sigma_2 = \sum_{k,s,v} W_{ks}^{(v)} p_s^{ss} \ln \frac{W_{ks}^{(v)} p_s^{ss}}{W_{sk}^{(v)} p_k^{ss}}; \tag{2.2.5}$$

where $k, s = 3, 4$. Noting that $\ln [W_{24}^{(v)}/W_{43}^{(v)}] = y_v$, one finds, in agreement with standard irrevesible thermodynamics [21], the following expression for the entropy production:

$$\sigma_2 = K_m R_m + K_e R_e = \alpha(y_l - y_r)(g_r - g_l) \geq 0 \tag{2.2.6}$$

With thermodynamics forces for matter and energy flow, K_m and K_e, given by

$$K_m \equiv -(\frac{\mu_r}{T_r} - \frac{\mu_l}{T_l}), K_e \equiv \frac{1}{T_r} - \frac{1}{T_l} \tag{2.2.7}$$

We stress that the corresponding matter and heat flow, given by

$$R_m = -J_r, R_e = -(\epsilon - \Delta)J_r \tag{2.2.8}$$

are proportional to each other. In other words, matter and heat flow are perfectly coupled and the condition for attaining both Carnot and Curzon-Ahlborn efficiency, is fulfilled [11,22]. We first discuss the case of equilibrium. Due to the perfect coupling, it is enough to stop one current, matter or energy, and the other one will automatically vanish. Under this condition, detaild balance is valid, $I_v = 0$ and $J_v = 0$. It is clear from eq. (2.1.24) and eq. (2.1.27) that the matter flux (hence also the energy flux) vanishes if and only if $f_l = f_r$,$g_l = g_r$ or equivalently, $x_l = x_r$, $y_l = y_r$.the efficiency then becomes equal to the

Carnot efficiency, cf.eq.(2.1.38), and the entropy production vanishes, $\sigma_1 = o$ and $\sigma_2 = 0$ (cf.eq.(2.2.2) and cf.eq.(2.2.6) respectively). Note that $x_l = x_r$, $y_l = y_r$ does not require that the thermodynamic forces F_m and F_e vanish separetly, i.e at this singular balancing point equilibrium does not require temprature and chemical potential to be identical in both reservoirs [7,8,11,22]

Chapter 3

Graphic interpretation of thermodynamic quantity

In this chapter we evaluate and explore the behaviors of heat flux and power as a function of a scaled energy parameter $\frac{\Delta}{\epsilon}$ characterizing the energy difference between the two levels by using graphs.

3.1 heat flux

Heat flux is the rate of heat energy transfered through a given surface.

Recall $x_r = \frac{\epsilon+\Delta-\mu_r}{T_r}$

$y_r = \frac{\epsilon-\Delta-\mu_r}{T_r}$

Substituting x_r, y_r, f_r, g_r in eq. (2.1.34) the steady state heat per unit time as a function of $\frac{\Delta}{\epsilon}$ becomes

$$\dot{Q}_r(\frac{\Delta}{\epsilon}) = \alpha\epsilon\left\{(\frac{\Delta}{\epsilon}+x)(\frac{1}{1+exp(10(x+\frac{\Delta}{\epsilon}))} - \frac{1}{1+exp(20(y+\frac{\Delta}{\epsilon}))}) + (-\frac{\Delta}{\epsilon}+x)(\frac{1}{1+exp(10(x-\frac{\Delta}{\epsilon}))} - \frac{1}{1+exp(20(y-\frac{\Delta}{\epsilon}))})\right\} \qquad (3.1.1)$$

where $x = 1 - \frac{\mu_r}{\varepsilon}$, $y = 1 - \frac{\mu_l}{\varepsilon}$.

The steady state heat per unit time when $\Delta = 0$ becomes

$$\dot{Q}_r(\Delta = 0) = 2\alpha\epsilon(x)(\frac{1}{1+exp(10(x))} - \frac{1}{1+exp(20(y))}). \qquad (3.1.2)$$

Then $\frac{\dot{Q}_r(\frac{\Delta}{\epsilon})}{\dot{Q}_r(\Delta=0)}$ is:

$$\frac{\dot{Q}_r(\frac{\Delta}{\epsilon})}{\dot{Q}_r(\Delta=0)} = \Bigg\{ (\frac{\Delta}{\epsilon}+x)(\frac{1}{1+exp(10(x+\frac{\Delta}{\epsilon}))} - \frac{1}{1+exp(20(y+\frac{\Delta}{\epsilon}))}) + (-\frac{\Delta}{\epsilon}+x)(\frac{1}{1+exp(10(x-\frac{\Delta}{\epsilon}))} - \frac{1}{1+exp(20(y-\frac{\Delta}{\epsilon}))}) \Bigg\} \quad (3.1.3)$$

The graph becomes

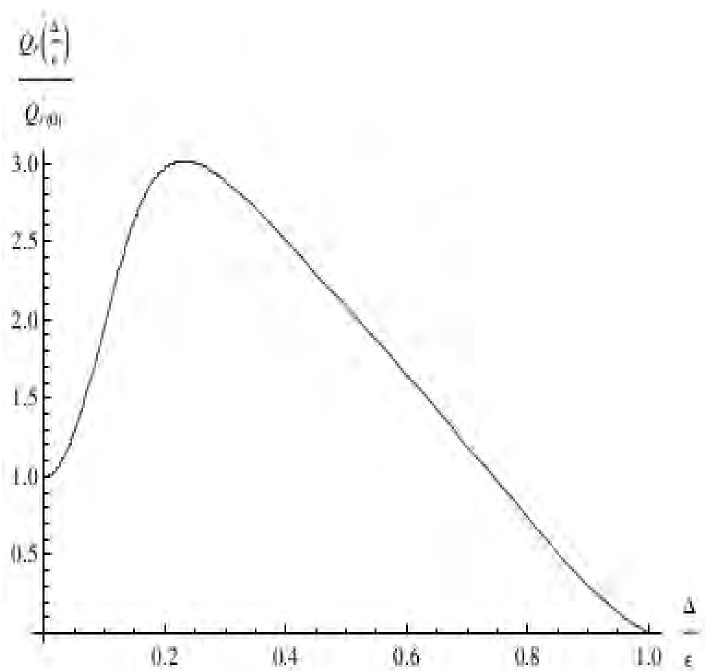

Figure 3.1: The ratio of total heat flux $\frac{\dot{Q}_r(\frac{\Delta}{\epsilon})}{\dot{Q}_r(\Delta=0)}$ from the hot reservoir at a temperature T_r as a function of $\frac{\Delta}{\epsilon}$ when x=0.99999 and y=0.1

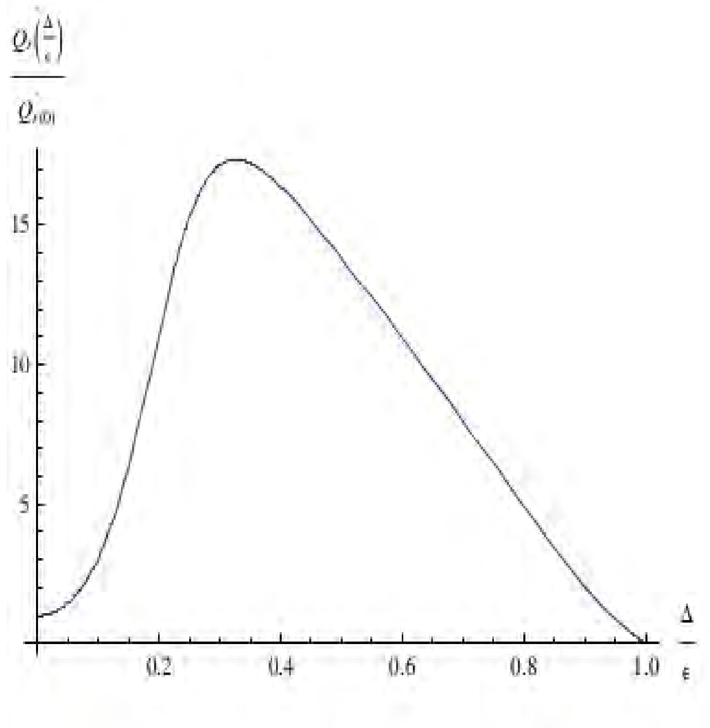

Figure 3.2: The ratio of total heat flux $\frac{\dot{Q}_r(\frac{\Delta}{\epsilon})}{\dot{Q}_r(\Delta=0)}$ from the hot reservoir at a temperature T_r as a function of $\frac{\Delta}{\epsilon}$ when x=0.99999 and y=0.2

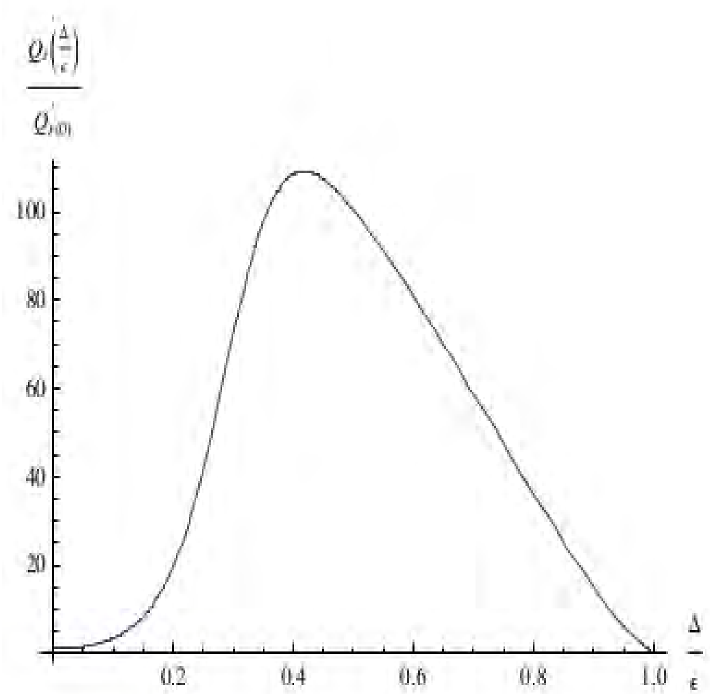

Figure 3.3: The ratio of total heat flux $\frac{\dot{Q}_r(\frac{\Delta}{\epsilon})}{\dot{Q}_r(\Delta=0)}$ from the hot reservoir at a temperature T_r as a function of $\frac{\Delta}{\epsilon}$ when x=0.99999 and y=0.3

From Fig. (3.1), (3.2), (3.3) and (3.4) which is the ratio of total heat flux as a function of $\frac{\Delta}{\epsilon}$. the heat flux getting in to the quantum dots increase when y is increase. Which means y is increase the chemical potential μ_l decrease but μ_l is grater than μ_r. If the chemical potential μ_l and μ_r are equal the power output will be zero. So our model is thermoelectric engine operates under irreversible process.

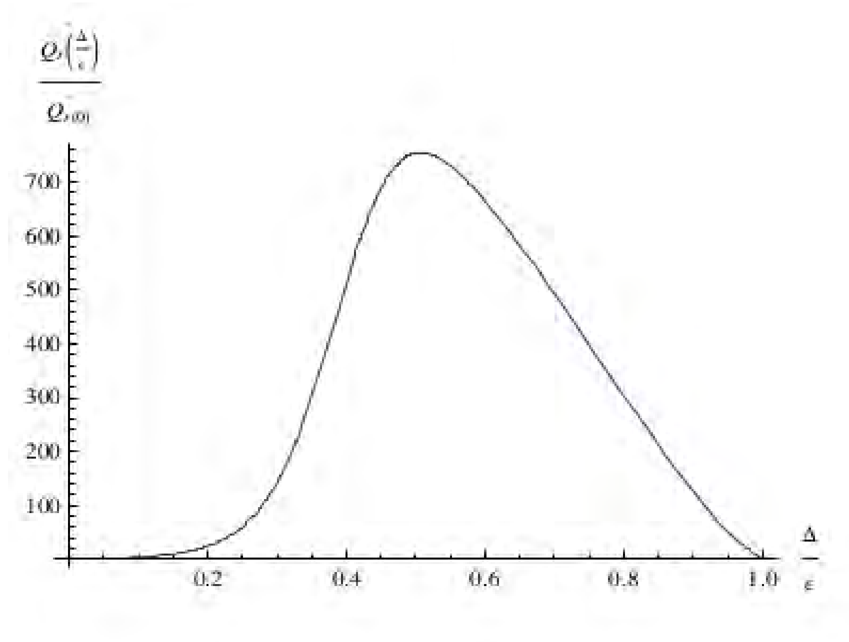

Figure 3.4: The ratio of total heat flux $\frac{\dot{Q}_r(\frac{\Delta}{\epsilon})}{\dot{Q}_r(\Delta=0)}$ from the hot reservoir at a temperature T_r as a function of $\frac{\Delta}{\epsilon}$ when x=0.99999 and y=0.4

3.2 Power

Power is the rate at which energy is transfered, used, or transformed.

The steady state work per unit time (power) as the function of $\frac{\Delta}{\epsilon}$

$$\frac{\dot{W}(\frac{\Delta}{\epsilon})}{\dot{W}(\Delta=0)} = \frac{1}{2(1/(1+exp(10x)) - 1/(1+exp(20y)))}\left[\frac{1}{1+exp(10(x+\Delta/\epsilon))} - \frac{1}{1+exp(20(y+\Delta/\epsilon))} + \frac{1}{1+exp(10(x-\Delta/\epsilon))} - \frac{1}{1+exp(20(y-\Delta/\epsilon))}\right] \tag{3.2.1}$$

The corresponding graph becomes

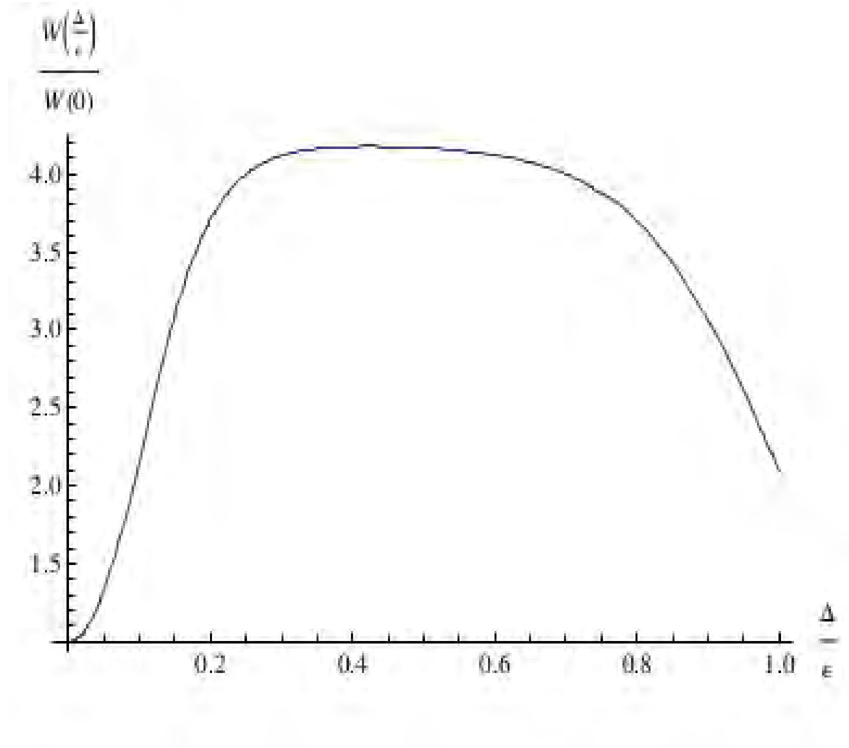

Figure 3.5: The net power out put $\frac{\dot{W}(\frac{\Delta}{\epsilon})}{\dot{W}(\Delta=0)}$ that delivers from the quantum dot as a function of $\frac{\Delta}{\epsilon}$ when x=0.99999 and y=0.1

.

From Fig.(3.5), (3.6),(3.7) and (3.8) which is the ratio of $\frac{\dot{W}}{\dot{W}(\Delta=0)}$ as a function of $\frac{\Delta}{\epsilon}$. The net power delivers from the quantum dot is increase when y is increase. Which means y is increase the chemical potential μ_l decrease but it is grater than μ_r. The input heat flux is increase the power output also increases.

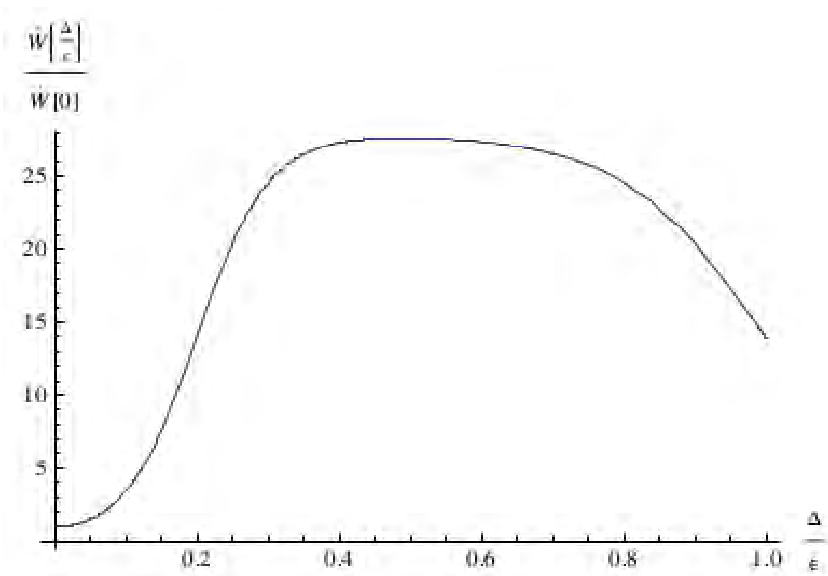

Figure 3.6: The net power out put $\frac{\dot{W}(\frac{\Delta}{\epsilon})}{\dot{W}(\Delta=0)}$ that delivers from the quantum dot as a function of $\frac{\Delta}{\epsilon}$ when x=0.99999 and y=0.2

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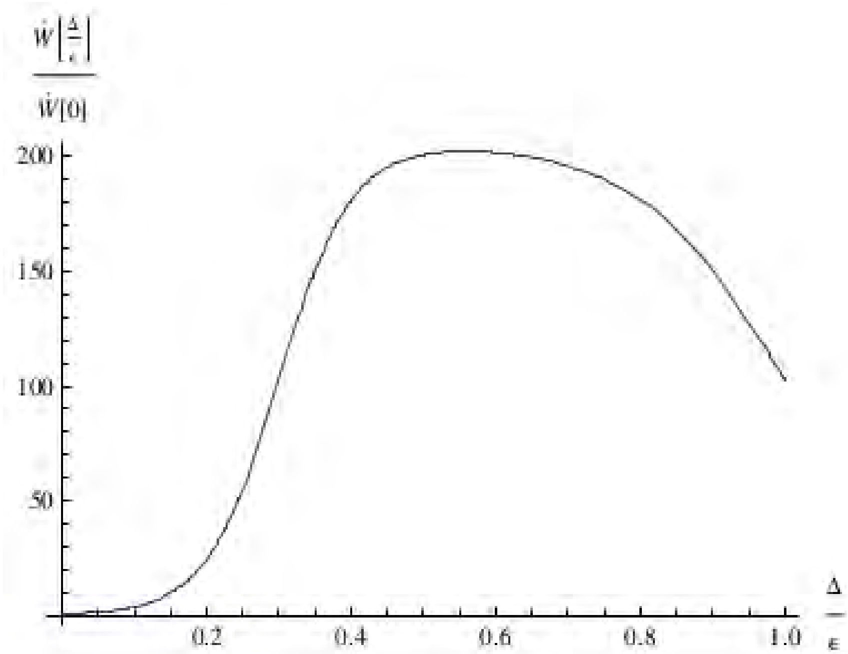

Figure 3.7: The net power out put $\frac{\dot{W}(\frac{\Delta}{\epsilon})}{\dot{W}(\Delta=0)}$ that delivers from the quantum dot as a function of $\frac{\Delta}{\epsilon}$ when x=0.99999 and y=0.3

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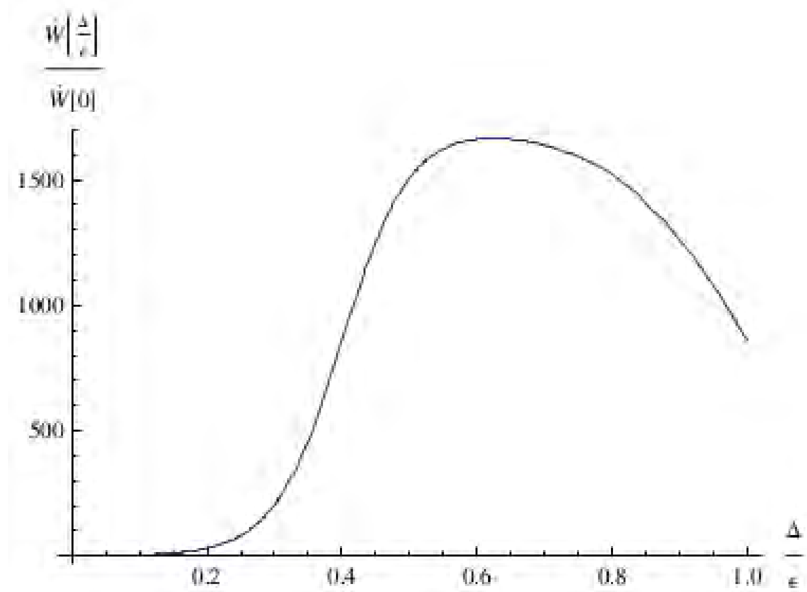

Figure 3.8: The net power out put $\frac{\dot{W}(\frac{\Delta}{\epsilon})}{\dot{W}(\Delta=0)}$ that delivers from the quantum dot as a function of $\frac{\Delta}{\epsilon}$ when x=0.99999 and y=0.4

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Chapter 4

Thermoelectric efficiency at maximum power

In this chapter we will see the values of maximum power and the result of efficiency at maximum power. The corresponding efficiency becomes the Curzon-Ahlborn efficiency up to quadratic term. We next turn to the operational condition for maximum power. For given temperature T_l and T_r, we search for the values of the scaled electron energy barriers x_l, x_r, y_l and y_r that maximize $\dot{W}$. We mean that the first derivative of power becomes zero. We find the following four equations. The first two equations are:

$$(f_l - f_r) + [x_r - (1-\eta_c)x_l]f_r^2 \exp(x_r) = 0 \tag{4.0.1}$$

$$(f_l - f_r) + [\frac{x_r}{1-\eta_c} - x_l]f_l^2 \exp(x_l) = 0 \tag{4.0.2}$$

and the second two equations are

$$(g_l - g_r) + [y_r - (1-\eta_c)y_l]g_r^2 \exp(y_r) = 0 \tag{4.0.3}$$

$$(g_l - g_r) + [\frac{y_r}{1-\eta_c} - y_l]g_l^2 \exp(y_l) = 0 \tag{4.0.4}$$

The first observation is that these equations depend only on the ratio of the two temperature. Second, while the equation involve transcedental relations, one obtains the following explicit result by simultaneous equations of equation (4.0.1 and 4.0.2) and the other simultaneous equations of equation (4.0.3 and 4.0.4) gives

$$(x_r - (1-\eta_c)x_l)\cosh(\frac{x_r}{2}) = (\frac{x_r}{1-\eta_c} - x_l)\cosh(\frac{x_l}{2}) \tag{4.0.5}$$

$$(y_r - (1-\eta_c)y_l)\cosh(\frac{y_r}{2}) = (\frac{y_r}{1-\eta_c} - y_l)\cosh(\frac{y_l}{2}) \tag{4.0.6}$$

From the above simultaneous equation we can get the values of x_l and y_l such as:

$$x_l = 2\ln[\frac{\cosh(x_r/2)}{\sqrt{1-\eta_c}} + \sqrt{\frac{\cosh^2(x_r/2)}{1-\eta_c} - 1}] \tag{4.0.7}$$

Substituting this result from equation(4.0.1) gives

$$x_r - \sqrt{2}\cosh(x_r/2)\sqrt{2\eta_c - 1 + cosh(x_r)} + 2(\eta_c - 1)\ln[\frac{\cosh(x_r/2) + \sqrt{\eta_c - 1 + \cosh^2(\frac{x_r}{2})}}{\sqrt{1-\eta_c}}] + \sinh(x_r) = 0 \tag{4.0.8}$$

and from the second simultaneous equation gives the value of y_l

$$y_l = 2\ln[\frac{\cosh(y_r/2)}{\sqrt{1-\eta_c}} + \sqrt{\frac{\cosh^2(y_r/2)}{1-\eta_c} - 1}] \tag{4.0.9}$$

Substituting this result from equation (4.0.3) gives

$$y_r - \sqrt{2}\cosh(y_r/2)\sqrt{2\eta_c - 1 + \cosh(y_r)} + 2(\eta_c - 1)\ln[\frac{\cosh(y_r/2) + \sqrt{\eta_c - 1 + \cosh^2(y_r/2)}}{\sqrt{1-\eta_c}}] + \sinh(y_r) = 0 \tag{4.0.10}$$

Since an analytic solution of this equation is not possible, we first turn to perturbative solutions for η_c close to the limiting values 0 (reservoirs of equal temperatures) and 1 (cold reservoir at zero temperature) and also find the numerical values of x_l^{mp} and x_r^{mp} for any values of η_c.

4.1 Solution when T_l approximately equal to T_r

When T_l and T_r are close to each other, η_c becomes very small and we turn to perturbative solution for η_{mp}. Within this range we can expand x_r^{mp} in powers of η_c,

$$x_r^{mp} = a_0 + a_1\eta_c + a_2\eta_c + \vartheta(\eta_c^3). \tag{4.1.1}$$

Inserting this equation in to equation(4.0.8) and expand the resulting equation in η_c. The coeffcients a_0, a_1, a_2, etc., are found recursively by solving order by order in η_c. At the first order, we find the transcedental equation.

$$\begin{aligned} a_0 &= 2\coth(a_0/2) \\ a_0 &= 2.39936 \end{aligned} \tag{4.1.2}$$

At second and third order in η_c. We find a_1 and a_2.

$$\begin{aligned} a_1 &= -a_0/4 \\ a_1 &= -0.599839 \end{aligned} \tag{4.1.3}$$

$$\begin{aligned} a_2 = \sinh(a_0)/[6(1 - \cosh(a_0))] \\ a_2 = -0.19946 \end{aligned} \tag{4.1.4}$$

Using the same steps expand y_r^{mp}

$$y_r^{mp} = b_0 + b_1\eta_c + b_2\eta_c^2 + \vartheta(\eta_c^3) \tag{4.1.5}$$

Substituting y_r^{mp} in equation(4.0.10) and expanding the resulting equations in η_c. The coefficients b_0, b_1, b_2, etc are found recursively by solving order by order in η_c. At the first order, we find the transcedental equation

$$\begin{aligned} b_0 &= 2\coth(b_0/2) \\ b_0 &= 2.39936 \end{aligned} \tag{4.1.6}$$

At second and third order in η_c, we find b_1 and b_2

$$b_1 = -a_0/4$$
$$b_1 = -0.599839 \tag{4.1.7}$$

$$b_2 = \sinh(a_0)/[6(1 - \cosh(a_0))]$$
$$b_2 = -0.19946 \tag{4.1.8}$$

The numerical value of a_0=b_0, a_1=b_1 and a_2=b_2. So, y_r=x_r and y_l=x_l. Then the fermi distribution becomes $f_l = g_l$ and $f_r = g_r$. Then Substituting all terms in the efficiency equation(equation(2.1.38)) is reduced in to

$$\eta^{mp} = 1 - (1 - \eta_c)\frac{x_l^{mp}}{x_r^{mp}} = 1 - (1 - \eta_c)\frac{y_l^{mp}}{y_r^{mp}} \tag{4.1.9}$$

Substituting x_r^{mp},y_r^{mp} and equation(4.0.7), equation(4.0.9) respectively in equation (4.1.9) leads to the following expanision of the efficiency at maximum power in the regime of small η_c:

$$\eta^{mp} = \frac{\eta_c}{2} + \frac{\eta_c^2}{8} + \frac{31}{400}\eta_c^3 + \vartheta(\eta_c^4) \tag{4.1.10}$$

4.2 Numerical solution for any temperature of the heat reservior

Before we evaluate numerically let us define a dimensionless quantity, τ, which is the difference between the hot and cold reservoir temperature with respect to the the cold reservior, i.e

$$\tau = \frac{T_r - T_l}{T_l} \tag{4.2.1}$$

From Eq.(4.0.8) and Eq.(4.0.10) we solve for the value of x_r^{mp} and y_r^{mp} for different values of τ numerically. Then we find the corresponding value of x_l^{mp} and y_l^{mp} from Eq.(4.0.7) and Eq.(4.0.9). Finally we substitute the values we get for x_r^{mp}, y_r^{mp}, x_l^{mp} and y_l^{mp} in Eq.(2.1.38) to find the efficiency at maximum power. From Fig.(4.1) which is the numerical solution for the efficiency at maximum power versus τ, we can observe that as τ goes to zero the efficiency at maximum power becomes zero. This is because when τ becomes very small the heat flux that is getting into the quantum dot becomes very small hence the efficiency is zero and as τ becomes large the efficiency at maximum power approaches to one because as τ increases the input power that the quantum dot receives increases which leads to an increases in efficiency.

Figure (4.2) shows as it is very close to the Curzon-Ahlborn efficiency when the Carnot efficiency is very small, but the Carnot efficiency is larger the maximum power is relative deviated. In the above expression tells as the Carnot efficiency is larger the engine operates becomes reversible, η_c is small the engine operates irreversible. Because of the corresponding efficency becomes Curzon-Ahlborn efficiency.

From figure(4.2), when the Carnot efficiency is zero, the efficiency at maximum power becomes zero. If the Carnot efficiency is approaches to one, the efficiency at maximum power approaches to one.

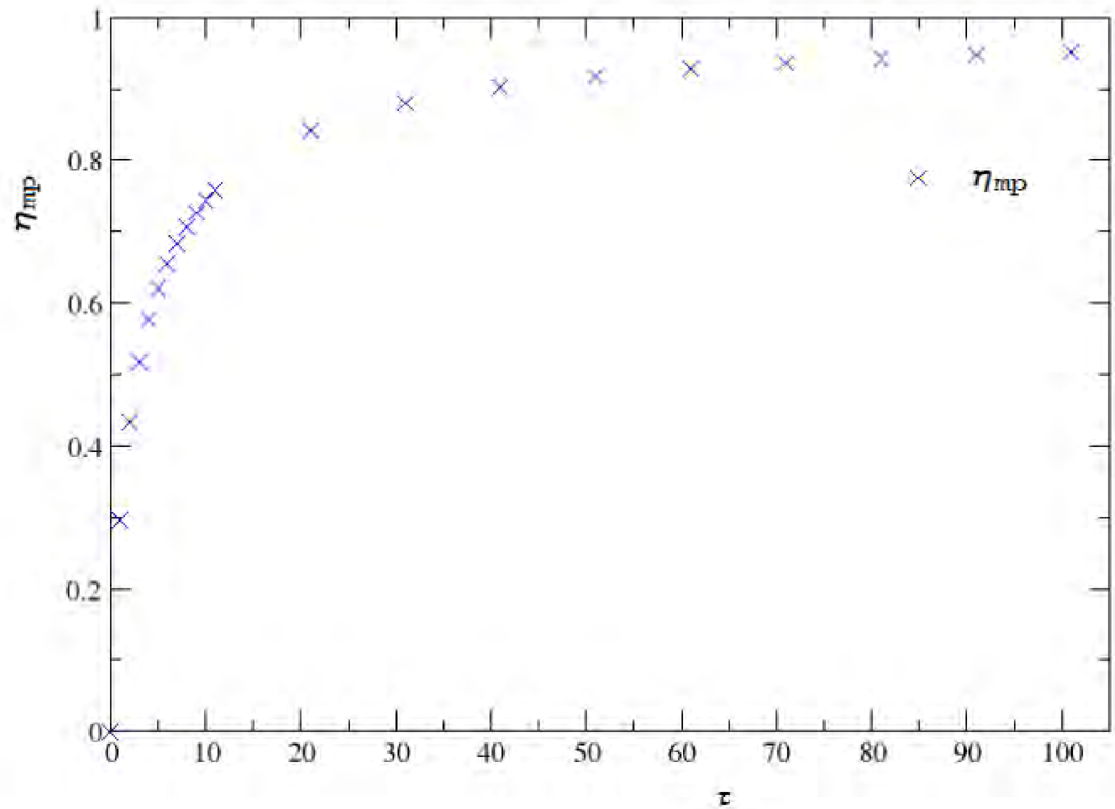

Figure 4.1: The plot of numerical value for efficiency at maximum power versus $= \frac{T_r - T_l}{T_l}$

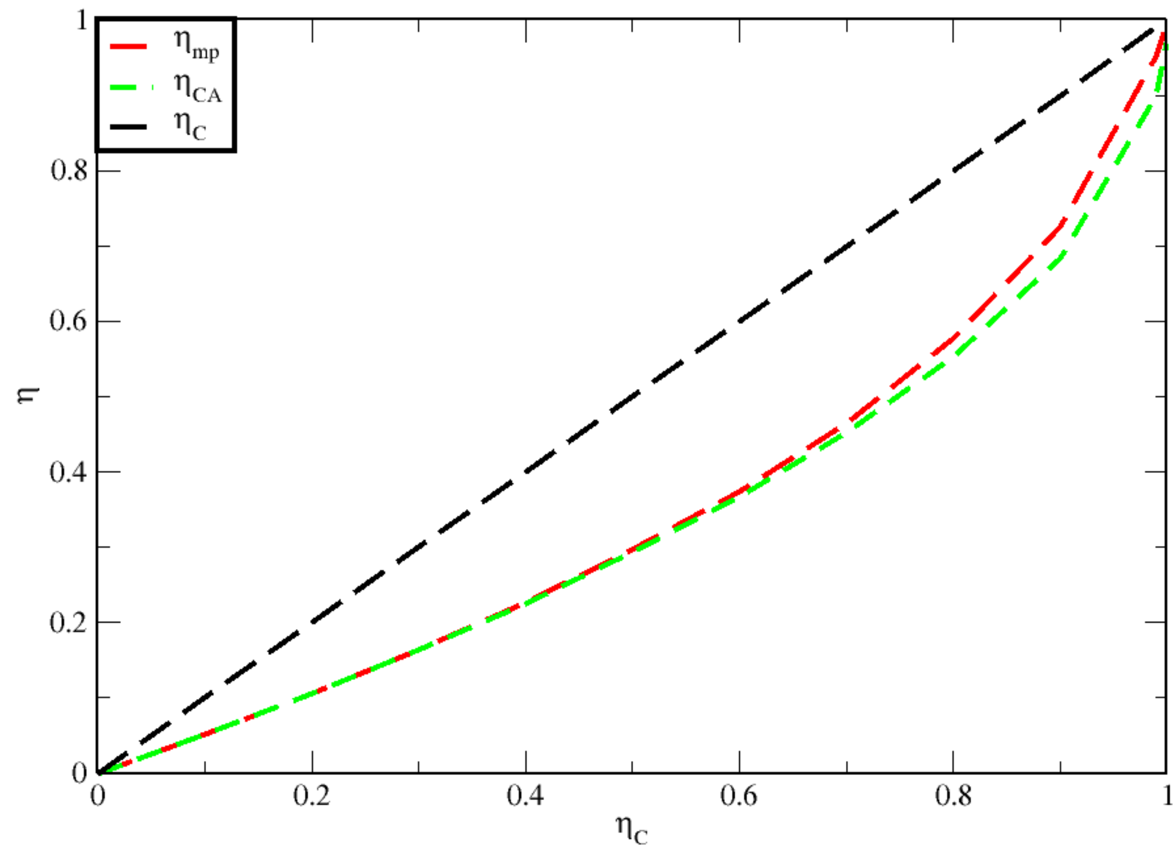

Figure 4.2: (color online)Efficiency at maximum power in a two quantum dot as a function of the carnot efficiency $\eta_c = 1 - \frac{T_l}{T_r}$(red color), as compared to Curzon-Ahlborn efficiency (green color) and Carnot efficiency (black color)

Chapter 5

Summary and Conclusion

In this thesis we have taken a simple model of a single level two quantum dots connected between two heat reservoirs working as heat engine. The simplicity of the model enabled us to get an analytic solution for the important quantities such as efficiency at maximum power.

To analyze the way energy is utilized by the engine, we started from the master equation and derived the efficiency, η, for the heat engine by first evaluating the heat flux extracted from the hot reservoir, $\dot{Q}_r$, heat flux dissipated to the cold reservoir, $\dot{Q}_l$, and power,$\dot{W}$ delivered by the quantum dot. Maximizing the efficiency with respect to our free parameters the scaled electron energy barriers, x_r, x_l, y_r and y_l. The efficiency at maximum power evaluated by two approaches such as analytical solution and numerical solution. When the temprature of thermal reservoirs gets closer to each other the coefficient of the linear term for the efficiency at maximum power is $\frac{1}{2}$.

In conclusion, we believe that our work has, for the first time, found an efficiency which is between the efficiency at maximum power (and also Curzon-Alhborn) and Carnot efficiency analytically, when the temperatures of the heat reservoirs are nearly equal.

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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.

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

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

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Signature:– – – – – – – – – – –