Optimal Performance Of Quantum Thermal Machine

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Certificate of Examination

This is to certify that the dissertation titled "Optimal Performance Of Quantum Thermal Machine" submitted by Mr. Tanmoy Pandit (MP16007) for the partial fulfilment of MS degree programme of the Institute, has been examined by the thesis committee duly appointed by the Institute. The committee finds the work done by the candidate satisfactory and recommends that the report be accepted.

Prof A	Prof A	Prof A
		(Supervisor)

Dated: April 30, 2019

Declaration

The work in this dissertation has been carried out by me under the guidance of Prof. Ramandeep Singh Johal at the Indian Institute of Science Educa- tion and Research Mohali.

This work has not been submitted in part or in full for a degree, a diploma, or a fellowship to any other university or institute. Whenever contributions of others are involved, every effort is made to indicate this clearly, with due acknowledgement of collaborative research and discussions. This thesis is a bonafide record of original work done by me and all sources listed within have been detailed in the bibliography.

Tanmoy Pandit

(Candidate)

Dated: April 30, 2019

In my capacity as the supervisor of the candidate's project work, I certify that the above statements by the candidate are true to the best of my knowledge.

Prof Ramandeep Singh Johal

(Supervisor)

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Abstract

The inexorable miniaturization of technologies stimulated the study of quantum thermodynamics. Quantum thermodynamics aims to explain the emergence of thermodynamic laws from quantum mechanics. The open quantum system is a benchmark to understand the non-equilibrium quantum system. Our main interest of this thesis is to understand the finite time thermodynamics study of the quantum thermal machine. Quantum thermodynamics provides a consistent explanation of quantum heat engines and refrigerators up to a single few-level system coupled to the environment. Once the environment is split into three (a hot, cold, and work bath), a heat engine can operate. The device converts the positive gain into power, with the gain obtained from population inversion between the components of the device. Reversing the operation transforms the device into a quantum refrigerator. We are devoted to find out the performance of the thermal machine at the high-temperature limit and find out the resemblance in the performance quantum thermal machine with finite time irreversible thermal device. Study of optimized performance helped us to understand the role of different parameters on the performance of the thermal machine.

In this work of optimal performance of three-level quantum refrigerator, we study a three-level quantum refrigerator operating at maximum χ criterion and cooling power. We study analytic expressions for the coefficient of performance (COP) under the assumptions of strong matter-field coupling and high bath temperatures. We also discuss the optimization of the χ criterion cannot be carried out for general due to **Casus Irreducibilis** of the cubic equation. The role of tight coupling assumption has been discussed in the context of two parameter optimization of χ criterion. In this model, we study the optimization of cooling power, and we describe why two parameter optimization of cooling power is not possible.

Chapter 1

Introduction

1.1 Prologue

In the last couple of decades, enormous progress has been done in miniaturization, nanotechnologies, and in general in the manufacturing and control of extremely small physical systems, some of which are composed of just a few atoms. We are now faced with the tormenting possibility of designing, implementing and using nano-machines, but because of their small size and quantum nature, their functioning and efficiency cannot be described by classical thermodynamics. Hence the need for developing quantum thermodynamics.

The general questions strike to mind: How do the laws of thermodynamics emerge from microscopic quantum mechanics? What are the requirements of a theory to describe quantum mechanics and thermodynamics within the same framework? What are the fundamental reasons for a trade-off between power and efficiency? What would be thermodynamics rules for quantum devices operating far from equilibrium? Can quantum phenomena like coherence, decoherence etc affect the performance of heat engines and refrigerators? What is then the effect of this counter-intuitive noise-induced quantum coherence on the performance quantum thermal machines? How is entropy production affected by it? Similarly, how would be quantum thermodynamic machine affected by entanglement? Can we use it as a resource for improving performances?

Quantum thermodynamics is devoted to unravel the connection between the laws of thermodynamics and their quantum origin. For many decades, the two theories developed separately. The work on the way to quantum thermodynamics has been stimulated after the seminal work of Scovil et al.[1] in which they showed the equivalence of the Carnot engine with three level Maser engine. With the development of quantum theory, the emergence of thermodynamics from quantum mechanics becomes a main issue. The two theories try to explain the same subject from different directions. To understand quantum thermodynamics better one has to deal with quantum dynamical behavior of the system. One needs to understand the theory of open quantum systems to study this kind of system. The Markovian master equation initiated by Lindblad and Gorini-Kossakowski-Sudarshan [2, 3] is one of the key resources of the theory of quantum thermodynamics. This formalism allows one to re-explain and justify the theory of finite time thermodynamics [4], which deals with thermodynamic processes taking place in finite time. So, an open quantum system is the generalized theoretical tool to understand the finite time quantum thermal machines.

Thermodynamics is one of the most successful and beautiful theories ever formulated. Though it was initially developed to deal with a macroscopic systems like steam engines, auto engines, etc. The seminal work of Carnot led Clausius [5] to formulate the second law of thermodynamics which introduced the concept of entropy. The Carnot engine has no practical importance as its output power is zero. A quantum mechanical model of heat engine or refrigerator allows us to incorporate dynamics into thermodynamics. In this thesis, we are mainly interested in an autonomous quantum heat engine and a quantum refrigerator. The autonomous quantum thermal machine is simultaneously connected with a hot and cold bath. This is different from Otto and Carnot cycles. Generally, a reciprocating cycle consists of four segments, two adiabats, where the working system is isolated from the environment, and two heat transfer segments, either isotherms for the Carnot cycle or isochores for the Otto cycle. The same cycles are then used as models for refrigerators.

In quantum thermodynamics, we generally address adiabats by time-dependent Hamiltonians. Typically, the external control Hamiltonian does not commute with the internal Hamiltonian. Infinitely slow operation is the necessary and sufficient condition for the quantum and thermodynamic adiabatic conditions. This condition is unable to generate finite output power. So we need to study quantum thermal machine at finite rates, and quantum dissipation comes into picture.

In quantum thermodynamics, an open quantum system is used to model the system-bath interaction. The LGKS generator is very useful to study the finite time quantum thermal machines. For finite power operation, the thermal transfer process is never allowed to equilibrate with the heat bath, which would take an infinite amount of time. Finally, maximum power output is obtained by optimizing over the time allocation on each of the segments of the cycle. The efficiency of the engine at maximum power can then be compared to the well-known results of finite-time thermodynamics. Although the mechanism of quantum thermal machine and classical thermal machine are very different, in the limit of high temperature limit, the quantum model harmonized with the results [6] with classical thermal machine which is the main focus of this thesis.

The main example of a continuous quantum engine is a three-level laser, whose efficiency is bounded by Carnot efficiency [1]. Many models of the quantum machine have been introduced for different types of continuous quantum engines, all consistent with the laws of thermodynamics [7, 8, 9]. The main example of a continuous refrigerator is laser cooling. In this context, it is obtained by reversing the operation of a three-level laser. In the journey of equivalence search of quantum and classical thermal machine, we also use semi-classical stochastic master equation which is based on probabilistic statistical mechanics, and end up with the same expression of efficiency at maximum power at the high temperature.

The thesis is divided in the following way: at first, we discuss about the open quantum system which is an important tool to study quantum thermal machine. Next, we explain a little bit about how to define heat and power for this kind of thermal machine. It is noted that the bath we consider in our work is a thermal bath and large bath (which means the degree of freedom of bath is very large). The state of the bath will not change through the thermodynamical protocol. In general, one can have micro bath then the above-mentioned assumption would no longer valid. The state of a bath will change even if the initial state is a thermal state. In scenario, one should seriously think about how to define heat and work. The definition that we have discussed here only valid for a large bath. In the next chapter, we introduce a three-level autonomous QHE model and studied finite time thermodynamics efficiency at maximum power. We also discuss some well known results of EMP in the context of linear irreversible thermodynamics. Then we are curious enough to study the three-level quantum refrigerator, and we have studied the optimal performance of the quantum refrigerator.

Chapter 2

Three-Level System As A Thermal Machine

2.0.1 Introduction

Thermodynamical study of quantum-optical systems has fascinated a lot of attraction after the experimental realization of masers and lasers. In the work of Scovil–Schulz-DuBois, they assumed the population of atomic level as Boltzmann distribution and they showed by a simple calculation that the engine's efficiency is limited by the Carnot efficiency. Alicki partitioned the total energy into two parts (heat and work) using time dependencies of the density operator and Hamiltonian operator. Later Geva and Koslof proved that the second law of thermodynamics is generally satisfied by careful consideration of the effect of the external field on the dissipative term [**?**]. In this chapter, we introduce three-level quantum System and how it can be used as a thermal machine (engine and refrigerator).

2.0.2 Quantum Three-Level as heat engine

A Three-level system can be used as a heat engine, and its efficiency is bounded by Carnot's efficiency. Let us introduce a three-level system as a contemporary example of a Carnot engine which is an amplifier as it amplifies input field. The principle of operation is to convert population inversion into output power in the form of light.

The hot bath which is at temperature T_h induces a transition between from the state $|g\rangle$ to excited state $|1\rangle$. When equilibrium is reached we can write $\frac{P_1}{P_g} = \exp\Big[-(\frac{\hbar\omega_h}{k_B T_h})\Big]$.

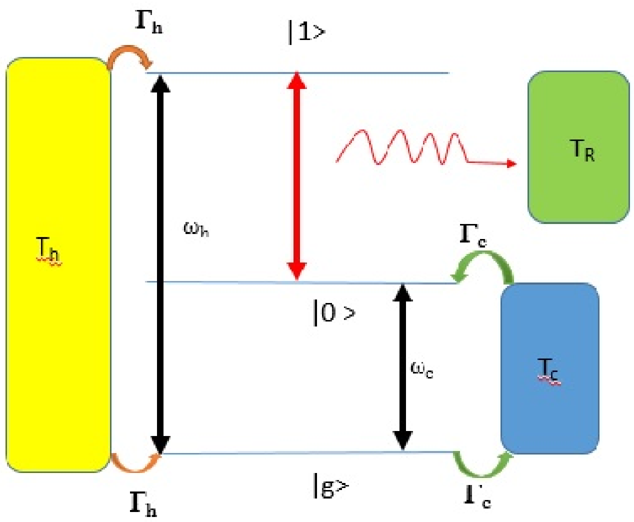

Figure 2.1: Three level quantum heat engine

Similarly for the cold bath which is at temperature T_c one can write similar expression $\frac{P_0}{P_g} = \exp\Big[-(\frac{\hbar\omega_c}{k_B T_c})\Big]$. The necessary and sufficient condition for amplification is positive gain or population inversion, defined by $P_g - P_1 > 0$, which leads to following condition

$$\frac{\omega_c}{\omega_h} \geq \frac{T_c}{T_h} \tag{2.1}$$

The efficiency of the heat engine is defined by

$$\eta = 1 - \frac{\omega_c}{\omega_h} \tag{2.2}$$

Using the equation 2.1 one can prove that $\eta \leq \eta_c$

The above description of the three-level amplifier is based on a quasi-static process. Real engines that produce power operate far from equilibrium conditions. Typically, their performance is restricted by different factors of dissipation like friction, heat transport, and heat leaks. One needs to understand the open quantum system formalism to study the real-life thermal quantum machine.

2.0.3 Quantum Three-Level as refrigerator

In a nutshell, refrigerators are engines operating in a regime where the heat flow is reversed. The three essential ingredients of a continuous three level refrigerator are a hot reservoir, a cold reservoir, and a working reservoir and it is simultaneously connected to the system as shown in the figure. In the refrigerator, heat is extracted from the cold reservoir and dumped into the hot reservoir. As in the heat engine, first and second law restricts the COP of a refrigerator. This induces transitions between level $|0\rangle$ and level $|1\rangle$. The population in level $|1\rangle$ then relaxes to level $|g\rangle$ by rejecting heat to the hot bath. The system then makes transitions from level $|g\rangle$ to level $|1\rangle$ by absorbing energy from a cold bath. There are dissipations corresponding to the hot and cold reservoir/bath respectively. Since this is a continuous thermal machine operating in the steady state condition, so the second law of thermodynamics has to be satisfied. By examining the heat engine model of Figure 1, one finds that if the

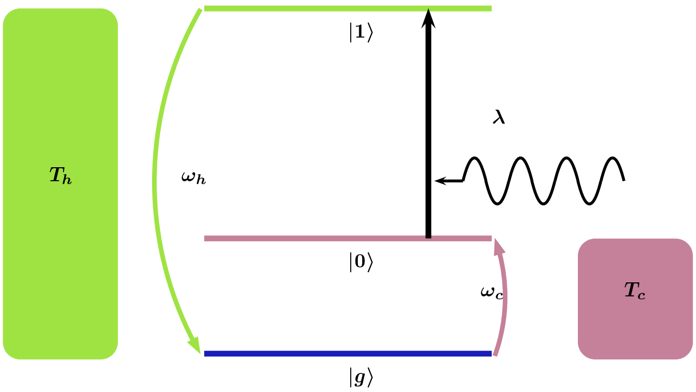

Figure 2.2: Three level quantum refrigerator

power direction is reversed, a refrigerator is generated, provided the gain is negative that is $P_g - P_1 < 0$. Assuming near equilibrium model one can get following condition

$$\frac{\omega_c}{\omega_h} \leq \frac{T_c}{T_h} \tag{2.3}$$

The coefficient of performance of refrigerator is given by

$$\epsilon = \frac{\omega_c}{\omega_h - \omega_c} \tag{2.4}$$

The coefficient of performance (COP) is always less than COP of Carnot's refrigerator (ϵ_c) i.e. $\epsilon \leq \epsilon_c$.

2.0.4 Conclusion:

Quantum heat engine is called the quantum amplifier as it amplifies the input field and quantum refrigerator called quantum attenuator as it reduces the input field. The key elements in a refrigerator are entropy extraction and ejection. This entropy ejection problem is enhanced at low temperatures. In the case of refrigerators, one has to take care of third law of thermodynamics. People have shown by adding one more level coherently with the third level one can enhance the efficiency of the heat engine. One can be interested in studying the noised induced performance in quantum thermal machine. It is nice to know that people of these days are realizing quantum thermal machine in the lab and observe the quantum effects on the thermal machine.

Chapter 3

Dynamics Of Open Quantum Systems

3.0.1 Introduction

An open quantum system is a system which interacts with another large quantum (the system having a large number of degrees of freedom) system environment/bath. As it interacts with the environment/bath, there is dissipation in the system. It is true indeed we can not prepare a quantum system which is isolated from the environment. Dynamics of a closed system can be represented by unitary time evolution, but in contrary, the dynamical evolution of an open system can not be represented by unitary time evolution. The tools of an open quantum system are extensively used in the field of quantum optics, quantum information, quantum thermodynamics, quantum statistics, etc.

Quantum Markov processes are the simplest dynamics of open systems. They are a direct generalization of the classical probabilistic concept of a dynamical semi-group to quantum process. In a simple man language, Markov process means the memoryless process that means the future is independent of the past, given the present. In classical probability theory there exist Chapman-Kolmogorov equation to study Markov process. Similarly, in quantum dynamical semigroup gives rise to a first order linear differential equation for the reduced density matrix, which is known as quantum Markovian master equation in Lindblad form. Most general quantum evolution should respect positively, hermiticity and trace-preserving conditions.

3.0.2 Dynamics of closed quantum systems

In non-relativistic quantum mechanics, state of a quantum system is represented by a state ket $|\psi\rangle$ in the Hilbert space $\mathcal{H}$. The time evolution of the closed quantum system is described by the Schrodinger equation:

$$-\frac{i}{\hbar}H(t)\left|\psi(t)\right\rangle = \frac{d\left|\psi(t)\right\rangle}{dt}, \tag{3.1}$$

where $H(t)$ is the Hamiltonian of the system and which is in general time-dependent. The formal solution of Schrodinger equation is given by

$$\left|\psi(t)\right\rangle = U(t,t_0)\left|\psi(t_o)\right\rangle, \tag{3.2}$$

where $U(t,t_0)$ is unitary time evolution operator satisfying the relation $U(t,t_0)^\dagger U(t,t_0) = U(t,t_0)U(t,t_0)^\dagger = I$, and $\left|\psi(t_o)\right\rangle$ is state of the system at some initial time t_0.

Substitution of Eq. (3.2) in Eq. (3.1) leads to an operator equation for $U(t,t_0)$:

$$-\frac{i}{\hbar}H(t)U(t,t_0) = \frac{\partial U(t,t_0)}{\partial t}, \tag{3.3}$$

subjected to the initial condition $U(t_0,t_0) = I$. For a closed and isolated quantum system, Hamiltonian is time independent and Eq. (3.3) is integrated to yield the following solution:

$$U(t,t_0) = e^{-iH(t-t_0)/\hbar}. \tag{3.4}$$

Nevertheless, in many physical cases, the system under consideration is driven by external time dependent forces such as time dependent electromagnetic fields. In such cases, the dynamics of the system is formulated in terms of a time dependent Hamiltonian $H(t)$, and the solution of Eq. (3.3) is represented by a time-ordered exponential,

$$U(t,t_0) = T_{\leftarrow}e^{-\frac{i}{\hbar}\int_{t_0}^{t} dsH(s)} \tag{3.5}$$

More generally, for a mixed state, state of the system is characterized by a density matrix ρ. Suppose at some initial time t_0, the state of the system is represented by the density matrix

$$\rho(t_0) = \sum_k p_k \left|\psi_k(t_0)\right\rangle \left\langle\psi_k(t_0)\right| , \tag{3.6}$$

where p_k are positive weights and $|\psi_k(t_0)\rangle$ are state kets, evolving in time according to Schrodinger equation (3.1). Therefore, at time t, the state of the system is given by

$$\rho(t) = \sum_k p_k U(t, t_0) \left|\psi_k(t_0)\right\rangle \left\langle\psi_k(t_0)\right| U(t, t_0)^\dagger, \tag{3.7}$$

which can be written as

$$\rho(t) = U(t, t_0)\rho(t_0)U(t, t_0)^\dagger. \tag{3.8}$$

Differentiating this equation with respect to time and simplifying a bit, we get the following equation of motion for the density matrix,

$$\frac{d\rho(t)}{dt} = -i\hbar[H(t), \rho(t)]. \tag{3.9}$$

Eq. (3.9) is known as Liouville-von Neumann equation and often written in a form analogous to classical Liouville equation

$$\frac{d\rho(t)}{dt} = \mathcal{L}(t)\rho(t), \tag{3.10}$$

where $\mathcal{L}$ is the Liouville super-operator, defined through the condition

$$\mathcal{L}(t)\rho(t) = -i\hbar[H(t), \rho(t)]. \tag{3.11}$$

In close analogy with Eq. (3.5), the formal solution of Eq. (3.10) is given by

$$\rho(t) = T_{\leftarrow} e^{\int_{t_0}^{t} ds \mathcal{L}(s)} \rho(t_0). \tag{3.12}$$

For a time independent Hamiltonian, $\mathcal{L}(t)$ is also time independent and thus we have

$$\rho(t) = e^{\mathcal{L}(t-t_0)} \rho(t_0). \tag{3.13}$$

3.0.3 Dynamics of open quantum systems

An open quantum system is a system S coupled to another quantum system B, usually very large as compared to system S, called environment. Thus it is a subsystem of the total system $S + B$, which is assumed to be closed and evolves according to unitary Hamiltonian dynamics. However, the dynamics of subsystem S cannot be represented in terms of unitary Hamiltonian dynamics due to its interaction with the environment.

Denoting Hilbert space of the system S and Hilbert space of the environment B by $\mathcal{H}_S$ and $\mathcal{H}_B$ respectively, the Hilbert space of the total system is given by the tensor product space $\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_B$. The total system+environment Hamiltonian $H(t)$ may be written as

$$H(t) = H_S \otimes I_B + I_S \otimes H_B + H_I(t), \tag{3.14}$$

where H_S is bare-Hamiltonian of the system S, H_B is the free-Hamiltonian of the

Figure 3.1: System-bath and Interaction

environment B. and $H_I(t)$ is the Hamiltonian of system-environment interaction, $I_{B,S}$ is the identity matrices of the bath and system respectively. Often in many physical situations, we need to solve the dynamics of the system S only. This can be done by tracing out the degrees of freedom of the environment by employing various analytical as well as numerical methods. If $\rho(t)$ represents the state of the combined total system, reduced density matrix ρ_S of the open quantum system is given by

$$\rho_S = tr_B[\rho], \tag{3.15}$$

where tr_B represents the partial trace over the degrees of freedom of the environment.

At time t, the reduce density matrix $\rho_S(t)$ of the open quantum system is obtained from the density matrix $\rho(t)$ of the total system by partially tracing out the degrees of freedom of the environment. Since $\rho(t)$ evolves unitarily, we have

$$\rho_S(t) = tr_B[U(t, t_0)\rho(t_0)U(t, t_0)^\dagger], \tag{3.16}$$

where $\rho(t_0)$ is density operator of the total system at some initial time t_0 and $U(t, t_0$ is the time-evolution operator of the total system. Similarly, by taking the partial trace over the environmental degrees of freedom on both sides of the Liouville-von Neumann equation for the total system, we may obtain equation of motion for the reduce density matrix ρ_S,

$$\frac{d\rho_S(t)}{dt} = -i\hbar[H(t), \rho(t)]. \tag{3.17}$$

3.0.4 Quantum dynamical semigroups

In general, it is challenging to solve the dynamics of the reduced system described by Eq. (3.17). However, when environmental correlation times are short, we may apply Markovian approximation to neglect memory effects and formulate the dynamics of the reduced system in terms of a quantum dynamical semigroup.

We are interested in the case when the the environment is in the equilibrium state and it is indeed a plausible assumption as environment is a quantum system having large number of degrees of freedom. Suppose that at initial time $t = 0$, state of the total system $S + B$ is prepared in an uncorrelated product state $\rho(0) = \rho_S(0) \otimes \rho_B$, where ρ_S and ρ_B represent initial state of the reduced system S and equilibrium state of the bath B, respectively. Then, there exists a quantum dynamical map $\Lambda(t)$, describing the evolution of reduced system S from the initial time $t = 0$ to some other time $t > 0$, such that

$$\rho_S(t) = \Lambda(t)\rho_S(0) \equiv Tr_B\left[U(t, 0)(\rho_S(0) \otimes \rho_B)U(t, 0)^\dagger\right]. \tag{3.18}$$

It can be shown that $\Lambda(t)$ is a convex-linear, completely positive and trace-preserving quantum operation.

As mentioned already, when the reservoir correlation times are much shorter as compared to the characteristic time scale of the system evolution, we may neglect the memory effects (Markovian approximation) in the reduced system dynamics. Under the condition of Markovian approximation, the quantum dynamical map $\Lambda(t)$ satisfy the following semigroup property:

$$\Lambda(t_1)\Lambda(t_2) = \Lambda(t_1 + t_2), \qquad t_1, t_2 \geq 0. \tag{3.19}$$

A *quantum dynamical semigroup* is a continuous, one-parameter family $\{\Lambda(t) \,|\, t > 0\}$ of dynamical maps ($\Lambda(0) = I$), satisfying the relation given in Eq. (3.19).

Given a quantum dynamical semigroup, there exists a time independent linear map $\mathcal{L}$, the generator of the semigroup, which allows up to represent the semigroup in exponential form:

$$\Lambda(t) = e^{\mathcal{L}t}. \tag{3.20}$$

This representation allows us to yield a first-order differential equation [see Eq. (3.18)] for the reduced density matrix $\rho_S(t)$,

$$\frac{d\rho_S(t)}{dt} = \mathcal{L}\rho_S(t). \tag{3.21}$$

This equation is known as Markovian quantum master equation. The generator $\mathcal{L}$ represents a super-operator, and may be considered as the generalization of the Liouville super-operator introduced in section 3.1.

3.0.5 Lindblad quantum master equation

We will concentrate on the special form of the master equation which is local in time. This form preserves the trace and positivity of the reduced density matrix $\rho_S(t)$. The main assumptions to derive quantum master equation are

- **Born approximation**: This approximation assumes that the coupling between the system and the reservoir is weak. $\rho(t) \approx \rho_S(t) \otimes \rho_B(0)$

- **Markov approximation**: This approximation assumes that the reservoir correlation time τ_B is much smaller than the relaxation time τ_R of the open system.
- **Rotating wave approximation**: This involves an averaging over the rapidly oscillating terms in the master equation. This approximation is valid when intrinsic time scale τ_S of the system is small compared to the relaxation time τ_R of the open system.

Lindblad and separately Gorini, Kossakowski and Sudarshan proved that the most general form of the generator $\mathcal{L}$ of the quantum dynamical semigroup is given by

$$\frac{d\rho_S(t)}{dt} = \mathcal{L}\rho_S = -i\hbar\,[H, \rho_S] + \sum_k \gamma_k \Big(A_k \rho_S A_k^\dagger - \frac{1}{2} A_k^\dagger A_k \rho_S - \frac{1}{2} \rho_S A_k^\dagger A_k \Big), \quad (3.22)$$

$$\equiv -i\hbar\,[H, \rho_S] + \mathcal{L}_{dis}\rho_S. \quad (3.23)$$

The above quantum master equation is known as the LGKS equation or Lindblad equation. Here, A_k are known as Lindblad operators, H is effective Hamiltonian of the system. The first term of the generator represents the unitary part of the dynamics generated by the Hamiltonian H. $\mathcal{L}_{dis}$ is known as the dissipator and represents the effect of the environment on dynamics of the reduced system. Generally, it induces non-unitary, dissipative dynamics.

3.0.6 Conclusion:

We will use the Lindblad quantum master equation in our work. This open quantum formalism is very useful to study the quantum dynamics of Quantum Heat Engine and Quantum Refrigerator. We mainly focused on the steady-state operation of the Quantum Machine. This would be very interesting to ask if we take a non-markovian thermal bath or if we take a different thermal bath like Fermionic Thermal bath, Squeezed Thermal Bath. We have studied Fermionic Thermal bath, and we will discuss in the next few chapters.

Chapter 4

Thermodynamics Of Bipartite System

4.0.1 Introduction

Since the early stages of the development of quantum physics, thermodynamics of quantum system has fascinated many physicists. According to the first law of thermodynamics, energy can be partitioned into heat and work. Differentiating between heat and work is a little tricky in quantum thermodynamics. In this section, we will discuss what is heat and how to define work in weak system-bath coupling scenario. In statistical mechanics, the entropy function which is based on density matrix and it is known as von Neuman entropy. Born also distinguished between heat and work in different quantum statistical systems. Spohn also defined a new entropy function called Sphon entropy and proved that it is always positive.Soon after Sphon's work, Alicki used Sphon's formalism to define work and heat for time-dependent Hamiltonian systems.

The main goal of this chapter is to establish the definition of heat and work for time-independent field and which we will be using in our three-level Quantum Heat Engine model(QHE) and Quantum Refrigerator model (QR). One think should be kept in mind that the definition of heat and work by Alicki is true for time-dependent external field. We will define at first the heat and work in quantum thermodynamics and after that we will define the heat and the work for a bipartite system which is very useful for our work.

4.0.2 Heat and work for a unipartite system

The master equation of the system coupled to the thermal reservoir is given by the following equation

$$\dot{\rho} = \mathcal{L}[\rho] = \mathcal{L}_h[\rho] + \mathcal{L}_d[\rho] \tag{4.1}$$

,Where the first part represents unitary evolution of the system and second part represents dissipative part which is in-general not unitary.

The average energy of the system is given by

$$< E >= Tr[\rho(\tau)H(\tau)] \tag{4.2}$$

Alicki has partitioned between the heat and work as follows

$$Q = \int_0^t Tr[\frac{d\rho(\tau)}{d\tau}H(\tau)]d\tau \tag{4.3}$$

$$W = \int_0^t Tr[\frac{dH(\tau)}{d\tau}\rho(\tau)]d\tau \tag{4.4}$$

The definitions mentioned above are classically motivated as the definition of work in classical thermodynamics is $dW = Fdq$, where F is the generalized force, and dq is generalized displacement. The quantum-mechanical definition also suggests that Hamiltonian of the system is changing which is a tuning parameter of the system like dq and that is why we have the first derivative of Hamiltonian, and ρ remains fixed in the definition of work. Once we can identify the work and the remaining one trivially becomes heat.

4.0.3 The definitions of heat and work for time dependent external field

The Schr$\ddot{o}$dinger picture:

The definition of heat and work as follows

$$\dot{Q} = Tr[\mathcal{L}_d[\rho^S]H^S] \tag{4.5}$$

$$P = \dot{W} = Tr[\rho^S \frac{\partial H^S}{\partial t}] \tag{4.6}$$

Note that in this case of Hamiltonian dynamics there is no heat involved, and if for the time-independent Hamiltonian, there is no work done by the system.

The Heisenberg picture:

The definition of heat and work in this picture is given by

$$\dot{Q} = Tr[\mathcal{L}_d[\rho^S]H^S] \tag{4.7}$$

$$P = \dot{W} = Tr\left[\rho^S \left(\frac{\partial H}{\partial t}\right)^S\right] \tag{4.8}$$

The Interaction picture:

Assume the following Hamiltonian of the system:

$$H(t) = H_o + V(t) \tag{4.9}$$

Where, H_o is the bare Hamiltonian of the system and V(t) is the coupling to some external degree of freedom.

The heat and work should be redefined to avoid consistency problem when one goes from Schr$\ddot{o}$dinger picture to Heisenberg picture. We define heat and work as follows:

$$Q = \int_0^t Tr[\frac{\partial \rho(\tau)}{\partial \tau} H(\tau)]d\tau \tag{4.10}$$

$$W = \int_0^t Tr[\frac{\partial H(\tau)}{\partial \tau} \rho(\tau)]d\tau \tag{4.11}$$

The above two definition is the same as the R. Alicki's definition[10] , here total derivative changed into partial derivative.

4.0.4 Power and heat for a bipartite system

The Hamiltonian of the bipartite system is given as:

$$H = H_A \otimes I_B + I_A \otimes H_B + V_{AB} \tag{4.12}$$

Where, I_A and I_B are the identity matrix of the subsystem A and B respectively. The definition of heat and power of the bipartite system as follows.

$$P_A = -\frac{i}{\hbar} Tr[\rho_{AB}[H_A, V_{AB}]] \tag{4.13}$$

$$\dot{Q}_A = Tr[\mathcal{L}_d[\rho_{AB}]H_A] \tag{4.14}$$

The above definitions of power and heat are very useful in the calculation of different quantities of the autonomous thermal machine. In this section, we have defined power and heat in quantum thermodynamics without going into more details as it is a very involved calculations. These definitions are very useful to study QHE and Quantum Refrigerator.

4.0.5 Conclusion

It is a really little bit tricky to identify work and heat accurately in quantum thermodynamics. One thing we should understand that work is fully deterministic quantity, but heat is not. There is randomness associated with heat. So there is entropy flow associated with heat, but in work, it is not. It should be noted that the definition of heat and work which we discussed in this section is valid only for weak system-bath coupling. Here bath which we consider is a large bath. These definitions of heat and work are very challenging for the case of micro-bath (like a bath containing two spins which are at a specific temperature T)

Chapter 5

Linear Irreversible Heat Engine

5.0.1 Introduction

Non-equilibrium thermodynamics deals with the phenomena that is not in thermal equilibrium. The non-equilibrium process deals with mainly transport phenomenon, chemical reaction, etc. It is extensively used to describe the different biological phenomenon, macroscopic process, etc. The study of non-equilibrium thermodynamics is significant as the systems we find in the practical world operate far from equilibrium. So, it is essential to understand the physics of the non-equilibrium process.

In this chapter, we will discuss the basic results of non-equilibrium heat engine. In our work, we deal with QHE model, and after taking the high-temperature limit, we got some well-known form of efficiencies expression which is well-established in the literature of finite time thermodynamics (FTT).

5.0.2 Irreversible Heat Engine Model

We know that the Carnot engine puts a theoretical upper bound on efficiency, but it is of no use as it requires infinite time to complete one cycle. The power output of the Carnot engine is zero. But in reality heat engines have a different kind of irreversibilities. For now, we will model the irreversible heat engine. Irreversibility can be either external or internal.

- **Endoreversible model:** For simplicity, we assume that there are no internal irreversibilities, like friction, dissipation are present in the system, and all the irreversibilities are external. That is for heat exchange between reservoir and engine and there must be some temperature difference as shown in the figure. To take into account external irreversibility, we use FTT. This could be understood well using CA model [?].

Under the CA model, the heat engine operates between two intermediate temperature as shown in figure 5.1(a). It takes $\dot{Q}_h$ heat from a hot reservoir and dumps $\dot{Q}_l$ heat to cold reservoir per second. We assume that the engine simultaneously connected with hot and cold bath and heat transfer follows Newton's law of cooling.Then,

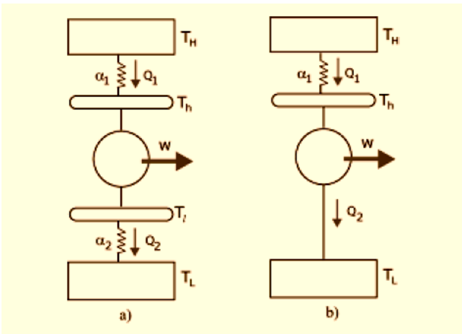

Figure 5.1: (a) Schematic of a heat engine with irreversibility at both ends of the reservoir and no internal irreversibility. (b) Schematic of heat engine with irreversibility only at the hotter end of the reservoir

$$\dot{Q}_h = K_h(T_H - T_h) \tag{5.1}$$

$$\dot{Q}_l = K_c(T_l - T_L) \tag{5.2}$$

where K_h and K_c is the heat conductance of the system. Now power extracted from the engine is P,

$$P = \dot{Q}_l - \dot{Q}_h \Rightarrow \dot{W} = K_h(T_H - T_h) - K_c(T_l - T_L) \tag{5.3}$$

where, t is the total cycle time. hence we see work is a function of intermediate temperature and it could be optimized according to them, but we need to take in consideration that these temperatures are not independent. As the engine is a endoreversible engine, so it must follows that entropy production rate internally is 0, therefore using equation (5.1) and (5.2),

$$\dot{S} = 0 \Rightarrow Q_l/T_l = Q_h/T_h \Rightarrow T_l/T_h = \frac{K_h(T_H - T_h)}{K_c(T_l - T_L)}. \tag{5.4}$$

Now using equation (5.3), power could be maximized and efficiency at maximum power(EMP) could be found.

Doing so we get that

$$EMP = (1 - \sqrt{T_c/T_h}) = 1 - \sqrt{1-\eta_c} = \eta_{CA}$$

Where, η_c is the Carnot-efficiency. The above result is very important and we found this result in many quantum heat engine model. In Ref [18] the authors proved that we get this η_{CA} for the case of left-right symmetry. We will show different QHE model leads to η_{CA} efficiency which is particularly interesting.

where η_c is Carnot efficiency, expanding it around $\eta_c = 0$ we get,

$$E.M.P = \eta_c/2 + \eta_c^2/8 + O(\eta_c^3) \tag{5.5}$$

The second term of the expansion is universal as proved in [18] and it is consequence of left-right symmetry.

- **Exoreversible model:** On the other hand of an endoreversible model, here we assume that all irreversibilities present in the system are internal, in the form of heat leaks or joule's heating, etc. and heat conductance to be infinite. Similar calculation as former case one could be do for exoreversible heat engine based on a particular model.

It can be shown in some Irreversible Heat Engine Model, the highest achievable efficiency at maximum power is $\eta = \frac{\eta_c}{2-\eta_c}$ [11]

5.0.3 Conclusion

In this section, we have discussed some standard results of EMP. This will be needed in the next few chapters. We have studied the three-level QHE model in the context of an open quantum system. Interestingly the result of EMP concurs with those results of EMP that we discussed in this chapter at the limit of high temperature. It is exciting to think about why these particular expressions appear in different models. This is the fantasy of thermodynamics. In Ref [19] author showed that the different expressions of EMP could be derived by using the concept Arithmetic Mean, Geometric Mean, and Pythagorean Mean.

Chapter 6

Applications

6.1 Three-Level Quantum Heat Engine

6.1.1 Introduction:

The study of the efficient conversion of various forms of energy to mechanical energy has been a topic of interest for more than a century. In this conversion process, a part of heat sucked from the hot bath is converted into work and the remaining heat dumped into cold bath and Carnot-efficiency puts a limit on the efficiency. A heat engine drives the natural current from a hot to a cold bath to generate power. Carnot engine is an idealized model of such kind, but it has no practical importance as it produces vanishing output power due to its reversible nature.

An autonomous heat engine is connected with hot, cold baths and power lead simultaneously. A continuous engine operates in an autonomous fashion attaining steady state mode of operation. The famous example of this kind of engine is the three-level quantum heat engine model that was introduced by Scovil and DuBois [1]. Later, Boukobza and Tannor showed in their seminal work [21], that three-level heat engine can be used as an amplifier or attenuator by controlling the population of different levels.

6.1.2 QHE Model:

The model consists of a three-level system continuously coupled to two thermal reservoirs and a single mode classical field. A hot reservoir at temperature T_h drives the transition between the ground level $|g\rangle$ and top level $|1\rangle$, whereas the transition between the intermediate level $|0\rangle$ and ground level $|g\rangle$ is constantly de-excited by a cold reservoir at temperature T_c. The power output mechanism is modeled by coupling the levels $|0\rangle$ and $|1\rangle$ to a classical single mode field. The Hamiltonian of the system

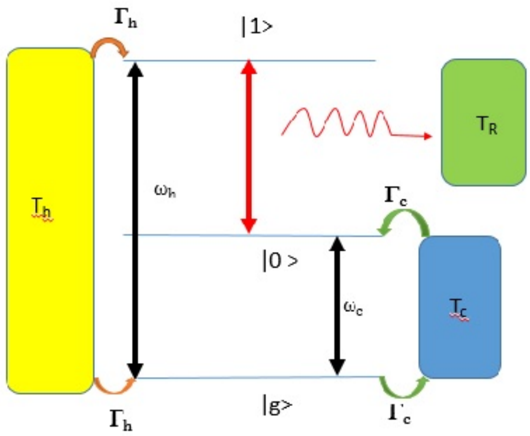

Figure 6.1: Three level Quantum Heat Engine Model.

is given by: $H_0 = \hbar \sum \omega_k |k\rangle\langle k|$, where the summation runs over all three states and ω_k represents the relevant atomic frequency. The interaction with the single mode lasing field of frequency ω, under the rotating wave approximation, is described by the semiclassical hamiltonian: $V(t) = \hbar\lambda(e^{i\omega t}|1\rangle\langle 0| + e^{-i\omega t}|0\rangle\langle 1|)$; λ is the field-matter coupling constant. The time evolution of the system is described by the following master equation:

$$\dot{\rho} = -\frac{i}{\hbar}[H_0 + V(t), \rho] + \mathcal{L}_h[\rho] + \mathcal{L}_c[\rho], \tag{6.1}$$

where $\mathcal{L}_{h(c)}$ represents the dissipative Lindblad superoperator describing the system-bath interaction with the hot (cold) reservoir and the commutator part represents the unitary evolution of the system:

$$\begin{aligned} \mathcal{L}_h[\rho] &= \Gamma_h(n_h+1)(2|g\rangle\langle g|\rho_{11} - |1\rangle\langle 1|\rho - \rho|1\rangle\langle 1|) \\ &\quad + \Gamma_h n_h(2|1\rangle\langle 1|\rho_{gg} - |g\rangle\langle g|\rho - \rho|g\rangle\langle g|), \end{aligned} \tag{6.2}$$

$$\begin{aligned}\mathcal{L}_c[\rho] &= \Gamma_c(n_c+1)(2|g\rangle\langle g|\rho_{00} - |0\rangle\langle 0|\rho - \rho|0\rangle\langle 0|) \\ &\quad +\Gamma_c n_c(2|0\rangle\langle 0|\rho_{gg} - |g\rangle\langle g|\rho - \rho|g\rangle\langle g|). \end{aligned} \tag{6.3}$$

Here Γ_h and Γ_c are the coupling constants with the hot and cold reservoirs respectively, and $n_{h(c)} = 1/(\exp\left[\hbar\omega_{h(c)}/k_B T_{h(c)}\right] - 1)$ is average occupation number of photons in hot (cold) reservoir satisfying the relations $\omega_c = \omega_0 - \omega_g$, $\omega_h = \omega_1 - \omega_g$.

In our model, it is possible to find a rotating frame in which the steady-state density matrix ρ_R is time independent. Defining $\bar{H} = \hbar(\omega_g|g\rangle\langle g| + \frac{\omega}{2}|1\rangle\langle 1| - \frac{\omega}{2}|0\rangle\langle 0|)$, an arbitrary operator A in the rotating frame is given by $A_R = e^{i\bar{H}t/\hbar}Ae^{-i\bar{H}t/\hbar}$. It can be shown that $\mathcal{L}_h[\rho]$ and $\mathcal{L}_c[\rho]$ remain unchanged under this transformation. Time evolution of the system density matrix in the rotating frame can be written as

$$\dot{\rho_R} = -\frac{i}{\hbar}[H_0 - \bar{H} + V_R, \rho_R] + \mathcal{L}_h[\rho_R] + \mathcal{L}_c[\rho_R] \tag{6.4}$$

Where, $V_R = \hbar\lambda(|1\rangle\langle 0| + |0\rangle\langle 1|)$.

For a weak system-bath coupling, the output power, heat flux and efficiency of the engine can be defined, using the formalism of Ref [2-3], as follows:

$$\begin{aligned} P &= -\frac{i}{\hbar}\mathrm{Tr}([H_0, V_R]\rho_R), & (6.5)\\ \dot{Q}_h &= \mathrm{Tr}(\mathcal{L}_h[\rho_R]H_0), & (6.6)\\ \eta &= -\frac{P}{\dot{Q}_h}. & (6.7)\end{aligned}$$

Time evolution of the density matrix elements reads as following:

$$\dot{\rho_{11}} = i\,\lambda\,(\rho_{10} - \rho_{01}) - 2\,\Gamma_h[\,(n_h+1)\,\rho_{11} - n_h\,\rho_{gg}\,] \tag{6.8}$$

$$\dot{\rho_{00}} = -i\,\lambda\,(\rho_{10} - \rho_{01}) - 2\,\Gamma_c[\,(n_c+1)\,\rho_{00} - n_c\,\rho_{gg}\,] \tag{6.9}$$

$$\rho_{gg} = 1 - \rho_{11} - \rho_{00} \tag{6.10}$$

$$\dot{\rho_{10}} = -[\,i\Delta + \Gamma_h(n_h+1) + \Gamma_c(n_c+1)\,] + i\,\lambda\,(\rho_{11} - \rho_{00}) \tag{6.11}$$

In this mode of operation, we are assuming that resonance mode of operation of laser, so one can safely put Δ=0. Putting the values of H_0, V_R and $\mathcal{L}_h[\rho_R]$, and calculating the traces appearing in right hand side of the Eqs. (6.5) and (6.6), the power and heat flux can be written as:

$$P = i\hbar\lambda(\omega_1 - \omega_0)(\rho_{01} - \rho_{10}) = i\hbar\lambda(\omega_h - \omega_c)(\rho_{01} - \rho_{10}), \tag{6.12}$$

$$\dot{Q}_h = i\hbar\lambda\omega_h(\rho_{01} - \rho_{10}), \tag{6.13}$$

where $\rho_{01} = \langle 0|\rho_R|1\rangle$ and $\rho_{10} = \langle 1|\rho_R|0\rangle$. Then, the efficiency is given by

$$\eta = 1 - \frac{\omega_c}{\omega_h}. \tag{6.14}$$

The positive power production condition implies that $\omega_c/\omega_h \geq T_c/T_h$. Hence $\eta \leq \eta_c$.

6.1.3 Maximizing Power:

Expression of power of the heat engine model is :

$$P = \frac{2\,\hbar(n_c - n_h)(\omega_c - \omega_h)\,\Gamma_c\,\Gamma_h}{(\Gamma_h + \Gamma_c + 3\,n_h\,\Gamma_h + 3\,n_c\,\Gamma_c)} \tag{6.15}$$

Let's introduce some new parameters $\gamma = \Gamma_h/\Gamma_c$, $\tau = T_c/T_h$ and c=ω_c/ω_h, At high temperatures, $n_{h,c} = k_B T_{h,c}/\hbar\omega_{h,c}$, the expression of power in high temperature limit is given by:

$$P = \frac{2(1-c)(1-c\tau)\gamma\hbar\Gamma_c\omega_h}{3c(\gamma + c\tau)} \tag{6.16}$$

Doing $\partial P/\partial c$=0, and fixing the ω_h, we get the following expression of efficiency:

$$\eta^{\omega_h}_{SSD} = \gamma^{-1}[\tau + \gamma - \sqrt{(\tau(1+\gamma)(\tau+\gamma)}] \tag{6.17}$$

The expression of power can also be written as follow:

$$P = \frac{2(1-c)(1-c\tau)\gamma\hbar\Gamma_c\omega_c}{3(\gamma + +c\tau)} \tag{6.18}$$

Similarly by doing $\partial P/\partial c$=0, and fixing the ω_c, we get the following expression of efficiency:

$$\eta^{\omega_c}_{SSD} = 1 - \frac{\tau}{\sqrt{(1+\gamma)(\tau+\gamma)} - \gamma} \tag{6.19}$$

6.1.4 Thermodynamics Bounds On efficiency:

In Ref[20], the authors obtained lower and upper bound of efficiency in limit $\gamma \to 0$ and $\gamma \to \infty$.

$$\frac{1-\tau}{2} \leq \eta^{\omega_h} \leq 1 - \sqrt{\tau} \tag{6.20}$$

$$1 - \sqrt{\tau} \leq \eta^{\omega_c} \leq \frac{1-\tau}{1+\tau} \tag{6.21}$$

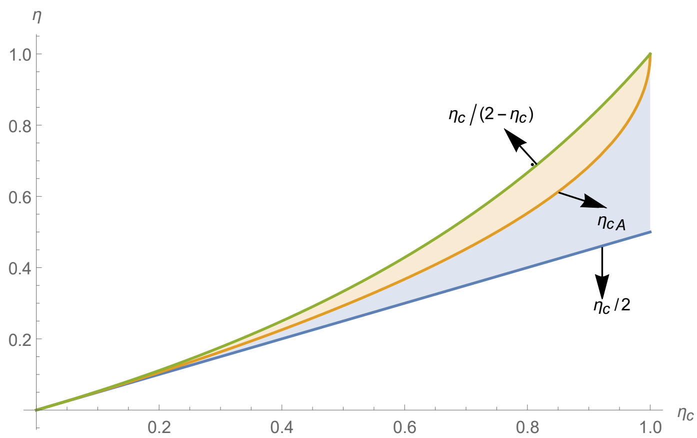

Figure 6.2: Plot of efficiency vs Carnot efficiency

6.1.5 Conclusion:

So, it is interesting to note that in the high temperature limit, our model of **QHE** leads to same form **EMP** as derived for any models of classical heat engine [29]. In the limit of extremely asymmetric dissipation, lower and upper bounds on the efficiency are obtained. η_{CA} serves as the upper bound in the former case and lower bound in the later case, thus separating the entire parameter regime of η into two parts.

6.2 Optimal Performance Of Three-Level Quantum Refrigerator

6.2.1 Introduction:

The thermal devices based on the principle of quantum thermodynamics are quantum heat engine, quantum refrigerator etc. In a nutshell, refrigerators are engines operating in a regime where the heat flow is reversed. In a series of papers [21, 22], Boukobza and Tannor formulated a new way of quantifying heat and work when the system-bath coupling is weak. They applied their analysis to a three-level atom continuously coupled to two baths and it is driven by coherent radiation. This induces transitions between level $|0>$ and level $|1>$. The population in level $|1>$ then relaxes to level $|g>$ by rejecting heat to the hot bath. The system then transitions from level $|g>$ to level $|0>$ by absorbing energy from a cold bath. There are dissipations corresponding to hot and cold reservoir respectively. Since this is a continuous thermal machine operating in the steady state condition, so second law of thermodynamics has to be satisfied. It has been shown in their paper that the maximum coefficient of performance (COP) is bounded by Carnot COP.

Back in 1989, the expression analogous to CA efficiency for refrigerators was first obtained by Yan and Chen by maximizing another optimization criterion, $\chi = \epsilon\dot{Q}_c$, which represents a trade-off between the the COP ϵ and CP $\dot{Q}_c$ of the refrigerator. The optimal form of the COP is given by $\epsilon_{CA} = \sqrt{1+\epsilon_C} - 1$, which also holds for many models of classical and quantum refrigerators . Recently, de Tomas and coauthors proved that χ figure of merit for refrigerators is true counterpart to the maximum power criterion for heat engines.

In this work, we study the optimal performance of a three-level quantum refrigerator. The choice of the model is motivated by the observation that it can be optimized for both CP and χ-criterion and yields model-independent expressions for lower and upper bounds on the COP in each case. Besides, the study of three level systems started the field of quantum thermodynamics. They have been employed to study

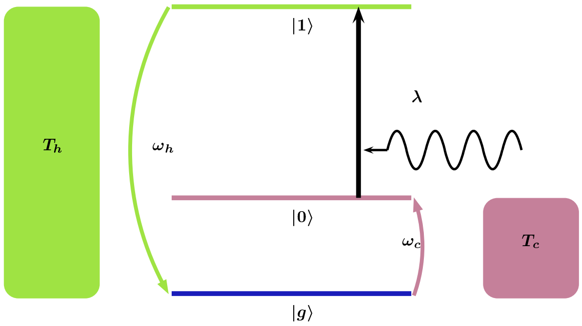

Figure 6.3: (Color online) Model of three-level laser refrigerator

quantum heat engines (refrigerators) and quantum absorption refrigerators

6.2.2 Three Level Quantum Refrigerator Model

The three basic ingredients of a continuous three level refrigerator are a hot reservoir, a cold reservoir and a work reservoir and it is simultaneously connected to the system as shown in the figure. In refrigerator, heat is extracted form cold reservoir and dumped into hot reservoir. As in the heat engine, first and second law impose restriction on the COP of a refrigerator. In a series of papers [21, 22], Boukobza and Tannor formulated a new way of quantifying heat and work when the system-bath coupling is weak. They applied their analysis to a three-level atom continuously coupled to two baths and it is driven by coherent radiation [22]. This induces transitions between level $|0\rangle$ and level $|1\rangle$. The population in level $|1\rangle$ then relaxes to level $|g\rangle$ by rejecting heat to the hot bath. The system then transitions from level $|g\rangle$ to level $|1\rangle$ by absorbing energy from a cold bath. There are dissipations corresponding to hot and cold reservoir respectively. Since this is a continuous thermal machine operating in the steady state condition, so the second law of thermodynamics has to be satisfied [23]. It has been shown in their paper that the maximum coefficient of performance (COP) is bounded by Carnot COP. The Hamiltonian of the system is given by: $H_0 = \hbar \sum \omega_k |k\rangle\langle k|$ where the summation runs over all three states and ω_k represents the relevant atomic frequency. The interaction with the single mode lasing field of frequency ω, under the rotating wave approximation, is described by the semiclassical hamiltonian: $V(t) = \hbar\lambda(e^{i\omega t}|1\rangle\langle 0| + e^{-i\omega t}|0\rangle\langle 1|)$; λ is the field-matter coupling constant. The most general time-independent dissipator generating a completely positive, trace-preserving and linear evolution was derived by Gorini, Kossakowski, Sudarshan and Lindblad [2, 3].

In the case of multiple, independent thermal environments, one can simply add their individuals contribution as

$$\mathcal{L}[\rho] = \mathcal{L}_h[\rho] + \mathcal{L}_c[\rho] \tag{6.22}$$

. Although, even the assumption of additivity (6.49) does not hold in general due to indirect interaction between the bath via the open system.The time evolution of the system is described by the following master equation:

$$\dot{\rho} = -\frac{i}{\hbar}[H_0 + V(t), \rho] + \mathcal{L}_h[\rho] + \mathcal{L}_c[\rho], \tag{6.23}$$

where $\mathcal{L}_{h(c)}[\rho]$ represents the dissipative Lindblad superoperator describing the system-bath interaction with the hot (cold) reservoir:

$$\begin{aligned} \mathcal{L}_h[\rho] &= \Gamma_h(n_h+1)(2|g\rangle\langle g|\rho_{11} - |1\rangle\langle 1|\rho - \rho|1\rangle\langle 1|) \\ &\quad + \Gamma_h n_h(2|1\rangle\langle 1|\rho_{gg} - |g\rangle\langle g|\rho - \rho|g\rangle\langle g|), \end{aligned} \tag{6.24}$$

$$\begin{aligned} \mathcal{L}_c[\rho] &= \Gamma_c(n_c+1)(2|g\rangle\langle g|\rho_{00} - |0\rangle\langle 0|\rho - \rho|0\rangle\langle 0|) \\ &\quad + \Gamma_c n_c(2|0\rangle\langle 0|\rho_{gg} - |g\rangle\langle g|\rho - \rho|g\rangle\langle g|). \end{aligned} \tag{6.25}$$

Here Γ_h and Γ_c are the Weisskopf-Wigner decay constants, and $n_{h(c)} = 1/(\exp\left[\hbar\omega_{h(c)}/k_B T_{h(c)}\right] - 1)$ is the average occupation number of photons in hot (cold) reservoir satisfying the relations $\omega_c = \omega_0 - \omega_g$, $\omega_h = \omega_1 - \omega_g$.

In our model, it is possible to find a rotating frame in which the steady-state density matrix ρ_R is time independent. Defining $\bar{H} = \hbar(\omega_g|g\rangle\langle g| + \frac{\omega}{2}|1\rangle\langle 1| - \frac{\omega}{2}|0\rangle\langle 0|)$, an arbitrary operator A in the rotating frame is given by $A_R = e^{i\bar{H}t/\hbar}Ae^{-i\bar{H}t/\hbar}$. It can be seen that $\mathcal{L}_h[\rho]$ and $\mathcal{L}_c[\rho]$ remain unchanged under this transformation. Time evolution of the system density matrix in the rotating frame can be written as

$$\dot{\rho_R} = -\frac{i}{\hbar}[H_0 - \bar{H} + V_R, \rho_R] + \mathcal{L}_h[\rho_R] + \mathcal{L}_c[\rho_R] \tag{6.26}$$

where $V_R = \hbar\lambda(|1\rangle\langle 0| + |0\rangle\langle 1|)$.

For a weak system-bath coupling, the input power, heat flux and coefficient of performance of the refrigerator can be defined, using the formalism of [22], as follows:

$$\begin{aligned} P &= \frac{i}{\hbar}\mathrm{Tr}([H_0, V_R]\rho_R), && (6.27)\\ \dot{Q}_c &= \mathrm{Tr}(\mathcal{L}_c[\rho_R]H_0), && (6.28)\\ \epsilon &= \frac{\dot{Q}_c}{P}. && (6.29)\end{aligned}$$

Plugging the values of H_0, V_R and $\mathcal{L}_h[\rho_R]$, and calculating the traces appearing in right hand side of the Eqs. (6.27) and (6.28), the power and heat flux can be written as:

$$P = i\hbar\lambda(\omega_1 - \omega_0)(\rho_{01} - \rho_{10}) = i\hbar\lambda(\omega_h - \omega_c)(\rho_{01} - \rho_{10}), \quad (6.30)$$

$$\dot{Q}_c = i\hbar\lambda\omega_c(\rho_{10} - \rho_{01}), \quad (6.31)$$

where $\rho_{01} = \langle 0|\rho_R|1\rangle$ and $\rho_{10} = \langle 1|\rho_R|0\rangle$. Then, the coefficient of performance is given by

$$\epsilon = \frac{\omega_c}{\omega_h - \omega_c}. \quad (6.32)$$

The coefficient of performance (COP) is always less than COP of Carnot's refrigerator (ϵ_c) i.e. $\epsilon \leq \epsilon_c$. For Carnot's refrigerator the cooling power vanishes and it also corresponds to zero entropy production.

6.2.3 Optimization Of χ Criterion

χ criterion is defined as the product of the the COP and CP of an refrigerator [24]. It has already been shown in many papers that it is a suitable figure of merit to study the optimal performance of classical as well as quantum refrigerators. We begin with plotting the 3D-graph of general expression for χ function as given in Eq. (6.53) (see Fig. 6.4). It is clear from Fig. 6.4 that global maximum exists in this case. But again it is not possible to obtain obtain the analytic expression for the the COP. Therefore, once again, we optimize the χ-criterion in the presence of strong matter-field coupling assuming high temperature limit, and obtain closed form expressions for the lower and upper bounds on the the COP. In the above-said regime, the expression for χ comes out to be

$$\chi = \epsilon\dot{Q}_c = \frac{\omega_c^2(\tau\omega_h - \omega_c)}{(\tau\omega_h + \gamma\omega_c)(\omega_h - \omega_c)}. \quad (6.33)$$

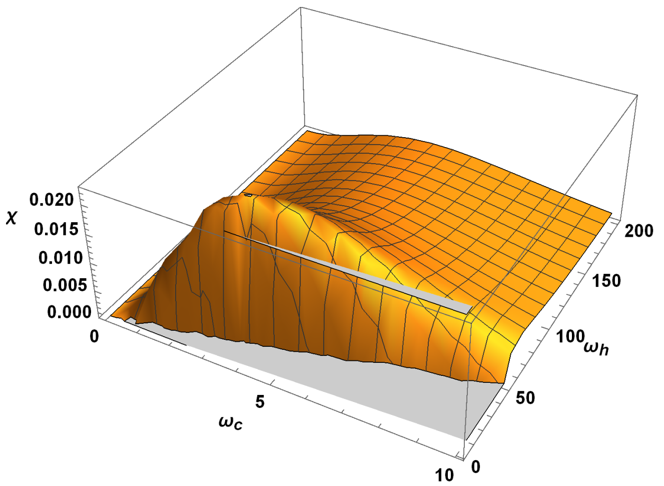

Figure 6.4: (Color online) 3D-plot of CP [Eq. (6.53)] in terms of control frequencies ω_c and ω_h for $\hbar = 1, k_B = 1, \Gamma_h = \Gamma_c = 1, \lambda = 1, T_h = 10, T_c = 2$.

First we try a two parameter optimization of the χ-criterion by setting $\partial\chi/\partial\omega_c = 0$ and $\partial\chi/\partial\omega_h = 0$. This gives the trivial solution, $\omega_h = \omega_c = 0$. Although in Fig. 3, we have shown the existence of global maximum of χ under general conditions, no such global maximum exists under the assumptions of strong-matter coupling and high temperatures. It can be reasoned as follows. While deriving Eq. (6.33), we have completely ignored the terms containing Γ_c and Γ_h as compared to λ. Mathematically, it can be viewed as $\lambda \to \infty$. Hence in this regime, the system has the affinity to couple to arbitrary high values of frequencies ω_c and ω_h, and as we go on increasing ω_c and ω_h, χ-criterion goes on increasing and optimal value of χ is never achieved.

Since two parameter optimization fails, we perform optimization of χ function alternatively with respect to ω_c (ω_h fixed) and ω_h (ω_c fixed). For fixed ω_c, setting $\partial\chi/\partial\omega_h = 0$, we have

$$\omega_c = \frac{\tau\omega_h\left(1 - \sqrt{(1+\gamma)(1-\tau)}\right)}{\gamma - \tau(1+\gamma)}. \tag{6.34}$$

Substituting Eq. (6.32) in Eq. (6.34), and writing in terms of Carnot the COP ϵ_C, we get following form of the COP at maximum χ-criterion

$$\epsilon^* = \frac{\epsilon_C}{1 + \sqrt{(1+\gamma)(1+\epsilon_C)}}. \tag{6.35}$$

Again ϵ^* is monotonic decreasing function of γ. Therefore we can obtain lower and upper bounds on the COP by putting $\gamma \to \infty$ and $\gamma \to 0$, respectively:

$$\epsilon_- \equiv 0 \leq \epsilon^* \leq \sqrt{1+\epsilon_C} - 1 \equiv \epsilon_{CA}. \tag{6.36}$$

Lower bound, $\epsilon_- = 0$, obtained here concurs with the lower bound of low-dissipation and minimally non-linear irreversible models of refrigerators. As mentioned earlier, upper bound, $\epsilon_{CA} = \sqrt{1+\epsilon_C} - 1$, obtained here was first derived for a classical endoreversible refrigerator. Under the conditions of tight-coupling and symmetric dissipation, ϵ_{CA} can also be obtained for the low-dissipation and minimally non-linear irreversible refrigerators. For a quantum Otto refrigerator, the COP emerges out to be equal to ϵ_{CA} in the classical limit (high temperature limit).

Next, we optimize χ with respect to ω_c while keeping ω_h constant at a fixed value (say k). In this case, optimization condition, $\partial\chi/\partial\omega_c$=0, yields the following equation

$$\frac{\omega_c\Big[\gamma\omega_c^3 + 2\omega_h(\tau-\gamma)\omega_c^2 - \tau\omega_h^2(3+\tau-\gamma)\omega_c + 2\tau^2\omega_h^3\Big]}{(\omega_c-\omega_h)^2(\gamma\omega_c+\tau\omega_h)} = 0. \tag{6.37}$$

Due to Casus irreducibilies (see Casus irreducibilies section), the roots of the above equation can only be expressed in complex radicals, although the roots are real actually. We can still obtain lower and upper bounds on the COP by solving Eq. (6.37) for the limiting cases $\gamma \to \infty$ and $\gamma \to 0$, respectively. For $\gamma \to \infty$, the the COP is evaluated at CA value, $\epsilon_{CA} = \sqrt{1+\epsilon_C} - 1$. For $\gamma \to 0$, we obtain the upper bound on the COP as $\epsilon_+ = (\sqrt{9+8\epsilon_C} - 3)/2$. Thus the COP lies in the range:

$$\epsilon_{CA} \leq \epsilon^* \leq \frac{1}{2}(\sqrt{9+8\epsilon_C} - 3). \tag{6.38}$$

Interestingly, ϵ_{CA} also appears as the lower bound for the optimization of a quantum model of refrigerator consisting of two n-level systems interacting via a pulsed external field [31]. However, the result reported in Ref. [31] was obtained in the linear response regime where $T_c \approx T_h$. In the same model, imposing the condition of equidistant spectra, ϵ_{CA} can be obtained as an upper bound in the classical regime for $n \to \infty$. The upper bound $\epsilon_+ = (\sqrt{9+8\epsilon_C} - 3)/2$ obtained here also serves as the upper limit on the efficiency for low-dissipation [25, 26] and minimally non-linear irreversible models [27]. Further, for a two-level quantum system working as a refrigerator, the

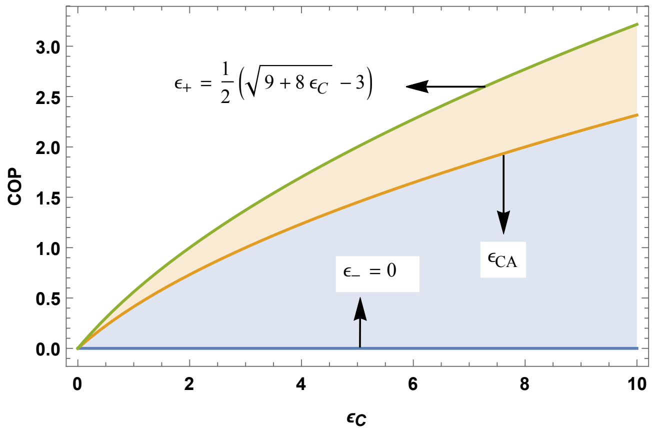

Figure 6.5: (Color online) Plot of the COP versus ϵ_C. ϵ_{CA} divides the parametric region of the the COP into two parts. For the optimization over ω_h, it serves as an upper bound whereas it is lower bound on the the COP for optimization over ω_c.

same upper bound can be derived in the high temperature regime.

6.2.4 Optimization Of Cooling Power

In this section, we optimize the CP $\dot{Q}_c$ of the refrigerator and obtain corresponding expression for the the COP. First, we start with the general case. The general expression for cooling the CP $\dot{Q}_c$ is derived in appendix A and is given by Eq. (6.52). We show the 3D-plot of CP with respect to ω_c and ω_h in Fig. 6.6. It is clear from the figure that a well defined local maxima on ω_c exists whereas there is no such local maxima on ω_h. In other words, CP is optimizable with respect to ω_c only. We have also tried plotting the same graph with a wide range of different values of the concerned parameters $(\Gamma_{c,h}, Tc, h, \lambda)$; the trend of the graph remains same and it does not change the main result. However in this case, the analytic expression for the the COP cannot be derived due to complicated equations.

In this section, we optimize the CP $\dot{Q}_c$ of the refrigerator and obtain corresponding expression for the the COP. First, we start with the general case. The general expression for cooling the CP $\dot{Q}_c$ is derived in section of steady state solution and is given by Eq. (6.52). We show the 3D-plot of CP with respect to ω_c and ω_h in Fig. 6.6. It is clear from the figure that a well defined local maxima on ω_c exists whereas there is no such local maxima on ω_h. In other words, CP is optimizable with respect to ω_c only. We have also tried plotting the same graph with a wide range of different values of the concerned parameters $(\Gamma_{c,h}, Tc, h, \lambda)$; the trend of the graph remains same and

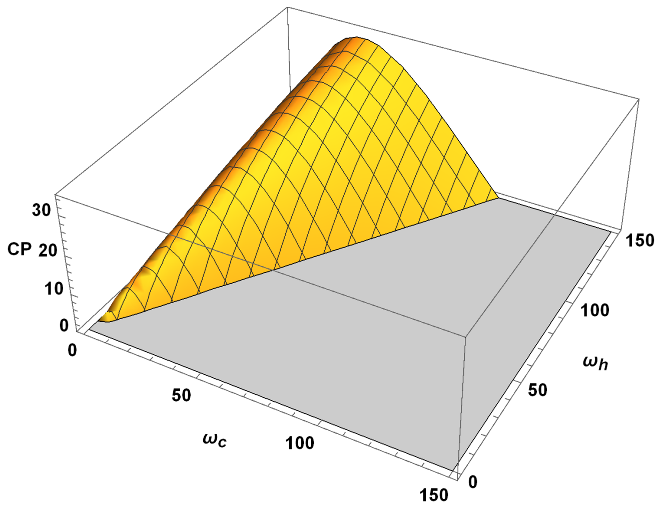

Figure 6.6: (Color online) 3D-plot of CP [Eq. (6.52)] in terms of control frequencies ω_c and ω_h for $\hbar = 1, k_B = 1, \Gamma_h = 3.4, \Gamma_c = 3.2, \lambda = 3, T_h = 60, T_c = 40$.

it does not change the main result. However in this case, the analytic expression for the the COP cannot be derived due to complicated equations.

In order to derive analytic expressions in closed form for the the COP, we will work in the high temperature regime and assume that matter-field coupling is very strong as compared to system-bath coupling ($\lambda \gg \Gamma_{h,c}$) [20]. While studying quantum heat engines or refrigerators, it is very common to work in high temperature regime as in this regime, quantum engines operate at CA efficiency and different models of quantum absorption refrigerators achieve their maximal performance. Moreover, in this regime, it is possible to obtain model-independent performance benchmarks for both quantum engines and refrigerators. In the high temperature limit, we set $n_h \simeq k_B T_h/\hbar\omega_h$ and $n_c \simeq k_B T_c/\hbar\omega_c$ and expression for CP is evaluated to be (see Steady state solution of density matrix equations)

$$\dot{Q}_c = \frac{\omega_c(\tau\omega_h - \omega_c)}{(\tau\omega_h + \gamma\omega_c)}, \tag{6.39}$$

where $\gamma = \Gamma_h/\Gamma_c$ and $\tau = T_c/T_h = \epsilon_C/(1+\epsilon_C)$. One can optimize $\dot{Q}_c$ in Eq. (6.39) in a local region at fixed ω_h by setting $\partial\dot{Q}_c/\partial\omega_c = 0$, leading to the following form of the COP at maximum cooling power

$$\epsilon^* = \frac{\epsilon_C}{1 + (1+\epsilon_C)\sqrt{(1+\gamma)}}. \tag{6.40}$$

We note that ϵ^* is monotonic decreasing function of γ. Therefore we can obtain lower and upper bounds on the the COP at maximum CP by putting $\gamma \to \infty$ and $\gamma \to 0$, respectively. Further, writing in terms of Carnot the COP ϵ_C, we have

$$0 \leq \epsilon^* \leq \frac{\epsilon_C}{2+\epsilon_C}. \tag{6.41}$$

These are the same bounds as obtained for the optimization of an minimally non-linear irreversible model [29] of refrigerator and an exoreversible thermoelectric refrigerator both operating in tight-coupling regime. Further $\epsilon^* = \epsilon_C/(2+\epsilon_C)$ can also be obtained for an endoreversible quantum refrigerator (see Eq. (14) in Ref.[15] for $d_c = 1$) operating at maximum CP.

6.2.5 Steady state solution of density matrix equations

Here, we solve the equations for density matrix in the steady state. Substituting the expressions for H_0, $\bar{H}$, V_0, and using Eqs. (6.24) and (6.25) in Eq. (6.26), the time evolution of the elements of the density matrix are given by following equations:

$$\dot{\rho}_{11} = i\lambda(\rho_{10} - \rho_{01}) - 2\Gamma_h[(n_h+1)\rho_{11} - n_h\rho_{gg}], \tag{6.42}$$

$$\dot{\rho}_{00} = -i\lambda(\rho_{10} - \rho_{01}) - 2\Gamma_c[(n_c+1)\rho_{00} - n_c\rho_{gg}], \tag{6.43}$$

$$\dot{\rho}_{10} = -[\Gamma_h(n_h+1) + \Gamma_c(n_c+1)]\rho_{10} + i\lambda(\rho_{11} - \rho_{00}), \tag{6.44}$$

$$\rho_{11} = 1 - \rho_{00} - \rho_{gg}, \tag{6.45}$$

$$\dot{\rho}_{01} = \dot{\rho}^*_{10}. \tag{6.46}$$

Solving Eqs. (6.42) - (6.46) in the steady state by setting $\dot{\rho}_{mn} = 0$ $(m, n = 0, 1)$, we obtain

$$\rho_{10} = \frac{i\lambda(n_h - n_c)\Gamma_c\Gamma_h}{\lambda^2[(1+3n_h)\Gamma_h + (1+3n_c)\Gamma_c] + \Gamma_c\Gamma_h[1+2n_h+n_c(2+3n_h)][(1+n_c)\Gamma_c + (1+n_h)\Gamma_h]}, \tag{6.47}$$

and

$$\rho_{01} = \rho^*_{10}. \tag{6.48}$$

Calculating the trace in Eq. (6.27), the input power is given by

$$P = i\hbar\lambda(\omega_h - \omega_c)(\rho_{10} - \rho_{01}), \tag{6.49}$$

Similarly evaluating the trace in Eq. (6.28), heat flux $\dot{Q}_c$ can be written as

$$\dot{Q}_c = \hbar\omega_c(2\Gamma_c[n_c\rho_{gg} - (n_c + 1)\rho_{00}]). \tag{6.50}$$

Using the steady state condition $\dot{\rho}_{00} = 0$ (see Eq. (6.42)), Eq. (6.50) becomes

$$\dot{Q}_c = i\hbar\lambda\omega_c(\rho_{10} - \rho_{01}). \tag{6.51}$$

Substituting Eqs. (6.47) and (6.48) in Eq. (6.51), we have

$$\dot{Q}_c = \frac{2\hbar\lambda^2\Gamma_c\Gamma_h(n_c - n_h)\omega_c}{\lambda^2[(1 + 3n_h)\Gamma_h + (1 + 3n_c)\Gamma_c] + \Gamma_c\Gamma_h[1 + 2n_h + n_c(2 + 3n_h)][(1 + n_c)\Gamma_c + (1 + n_h)\Gamma_h]}. \tag{6.52}$$

Expression for χ-criterion, $\chi = \epsilon\dot{Q}_c$, is given by

$$\chi = \frac{2\hbar\lambda^2\Gamma_c\Gamma_h(n_c - n_h)\omega_c^2}{\lambda^2(\omega_h - \omega_c)[(1 + 3n_h)\Gamma_h + (1 + 3n_c)\Gamma_c] + \Gamma_c\Gamma_h[1 + 2n_h + n_c(2 + 3n_h)][(1 + n_c)\Gamma_c + (1 + n_h)\Gamma_h]} \tag{6.53}$$

As for refrigerators, $n_c > n_h$, $\dot{Q}_c, \chi > 0$.

6.2.6 Casus Irreducibilis

In algebra, casus irreducibilis arises while solving a cubic equation. The formal statement of the casus irreducibilis is that if a cubic polynomial is irreducible with rational coefficients and has three real roots, then the roots of the cubic equation are not expressible using real radicals and thus, one must introduce expressions with complex radicals, even though the resulting expressions are actually real-valued. It was proven by P. Wantzel in 1843. Using the discriminant D of the irreducible cubic equation, one can decide whether the given equation is in casus irreducibilies or not, via Cardano's formula. The most general form of Cubic equation is given by

$$ax^3 + bx^2 + cx + d = 0 \tag{6.54}$$

where a, b, c, d are real.

The discriminant D is given by: $D = 18abcd - 4b^3d + b^2c^2 - 4ac^3 - 27a^2d^2$. Depending upon the sigh of D, following three cases arise:
(a) $D < 0$, the cubic equation has two complex roots, so casus irresucibilies does not apply.
(b) $D = 0$, all three roots are real and expressible by real radicals.
(c) $D > 0$, three are three distinct real roots. In this case, a rational root exists and can be found using the rational root test. Otherwise, the given polynomial is casus irreducibilis and we need complex valued expressions to express the roots in radicals.

In our case, in order to solve Eq. (6.37), we have to solve the following cubic equation

$$\gamma\omega_c^3 + 2\omega_h(\tau - \gamma)\omega_c^2 - \tau\omega_h^2(3 + \tau - \gamma)\omega_c + 2\tau^2\omega_h^3 = 0. \tag{6.55}$$

The discriminant D of the above equation is given by

$$D = 4\omega_h^6(1 + \gamma)(1 + \tau)[3\gamma^2(3 - \tau) + \gamma^3 + 9\gamma\tau + 3\gamma\tau^2 + 9\tau^2(1 - \tau)]. \tag{6.56}$$

Since the parameters ω_h, γ, τ are positive and $\tau < 1$; $D > 0$. So polynomial in Eq. (6.55) presents the case of casus irreducibilies.

6.2.7 Conclusion

In this work, we have studied the optimal performance of a three-level atomic system working as a refrigerator. To optimize its performance, we have chosen two different target functions: CP and χ-criterion. Although, in many classical and quantum models of refrigerator, CP is not a good figure of merit to optimize; in our model, it is well behaved function and we have obtained analytic expressions for lower and upper bounds on the COP already derived for some models of classical and quantum refrigerators. However, we notice that the CP is optimizable only with respect to the control frequency ω_c and thus, we can perform optimization in local region only. In contrast to the behavior of CP, χ-criterion shows global maximum which makes it more well behaved and more suitable figure of merit to study the optimal performance of refrigerators. In high temperature and strong-coupling regime, we have alternatively performed maximization of χ-criterion with respect to ω_h (ω_c fixed) and ω_c (ω_h fixed). In both the cases, we were able able to obtain the lower and upper limits on the the COP, already well known in the optimization literature of refrigerators. As Fig. 4 indicates, ϵ_{CA} separates the entire parameter region of ϵ^* into two parts. Refrigeration experiments with three level masers have already been carried out [1]. With the current status of technological advancements, three-level refrigerator can be tuned experimentally to achieve its optimal performance.

Chapter 7

Epilogue

In this thesis, we have mainly discussed the QHE model in the context of the master equation. In the first part, we have discussed the QHE with the bosonic type of reservoir, and we have analyzed the optimal performance of the QHE mainly in the regime of high temperature. The quantum master equation respects the completely positive dynamics which is the main ingredient to derive the quantum master equation and all the system operators can be written in terms of **kraus Operator** representation. In the limit of high-temperature, we checked the form of efficiency leads to some well-known form of efficiency's that are very well-known in the literature of finite time thermodynamics. In the second part we have played with bath spectral density, and we have also shown that for asymmetric spectral bath density case, we found the famous **CA** efficiency. After that, we have analyzed the same QHE model in the presence of the fermionic reservoir. Unfortunately, this is not solvable for the general case. We derived efficiency for some special cases. This also showed some important, interesting results, like it gives Carnot efficiency at symmetric dissipation case. In the last section, we have used stochastic master equation formalism in the model that has been introduced in the first section. We observed that we have the same bound on efficiency as derived from quantum master equation formalism although the general expressions of power are different in two formalisms. We then described the optimal performance of the three-level quantum refrigerator.

We are now dealing with the tantalizing possibility of enhancing both the performance and power of heat engines and quantum refrigerators. It has been shown that the squeezed-thermal, and other types of engineered non-equilibrium environments are capable of increasing the performance of heat engine and quantum refrigerator. One can study the performance of the same three-level quantum thermal machine in a different environment like the fermionic environment, squeezed-thermal environment. The main challenge lies in the implementation of this device for practical applications to quantum technologies. Recently various experimental setups have been implemented to realize the quantum heat engine and quantum refrigerator in different systems, including superconducting circuit, nanomechanical oscillator, quantum dots, atom-cavity system, trapped ions and optomechanics.

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