Optimizing the performance of a quantum many body continuous heat engine using CRAB

Shishira Mahunta

A dissertation submitted for the partial fulfilment of BS-MS dual degree in Science

Department of Physical Sciences

Indian Institute of Science Education and Research, Berhampur

May,2022

DECLARATION

This is to clarify that this dissertation entitled **"Optimizing the performance of a quantum many body continuous heat engine using CRAB"** submitted towards the Partial fulfilment of BS-MS dual degree programme at the Indian Institute of Science Education and Research, Berhampur represents project work carried out by **Shishira Mahunta** at the Indian Institute of Science Education and Research under the supervision of **Dr. Victor Mukherjee**, Assistant professor, Department of Physical Sciences, during the academic year 2021-2022.
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.

Shishira Mahunta.

Shishira Mahunta

(Candidate)

Dated: May 18, 2022

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.

Victor Mukherjee

Dr. Victor Mukherjee

(Supervisor)

CERTIFICATE OF EXAMINATION

This is to certify that the dissertation titled **"Optimizing the performance of a quantum many body continuous heat engine using CRAB"** submitted by **Shishira Mahunta** (**Reg. No. MS17096**) for the partial fulfilment of BS-MS dual 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.

Dr. Victor Mukherjee
[Supervisor]

Prof. S.N. Mishra
[Committee member]

Dr. Ujjal Kumar Dey

[DUGC, Physical Science Department]

Date

Prof. S.N. Mishra

[HoD, Physical Science Department]

Date

May, 2022

ACKNOWLEDGEMENT

I would like to convey my deepest gratitude to Dr. Victor Mukherjee for not only giving me the opportunities to carry out my MS research project under his supervision but also for the valuable guidance, constant support and encouragement during my MS project. His guidance and inspired lectures on quantum thermodynamics and open quantum system played a major role for the successful completion of my MS project. I would also like to thank Dr. Noufal for the fruitful discussion during my project. I would also like to thank my friend Durga, Rishav, Shiva and Gyatri for being there for me in my all ups and downs. Finally I would like to thank my parents and my family for their support and never ending love.

ABSTRACT

We study the detail thermodynamical description of a periodically driven continuous quantum heat engine with working medium as TLS and non-interacting indistinguishable multi-spin. In case of the multi-spin heat engine the atoms are collectively interacting with the bath, hence bath creates coherence in system which enhances the performance of the engine. We use quantum control technique to optimize the performance of the single-spin continuous engine. Optimization of the performance of the many-body heat engine can be expected to take long time owing to the large dimension of the corresponding Hilbert space. However we show that the performance of the many body quantum heat engine can be improved significantly using the optimal pulse for single-spin quantum heat engine whose reduced density matrix dynamics follow similar Landblad master equation to the many body engine.

Keywords: Quantum thermodynamics, Open quantum system, Quantum technology. Quantum control

Contents

List of Figures

Chapter 1

Introduction

One of the major aims of the field of quantum technologies is designing optimal quantum thermal machines through quantum control. In my thesis , we aim to focus on this problem, by engineering high-performing single and many-body continuous quantum heat engines through the chopped random basis (CRAB) numerical optimization algorithm[1][2]. The continuous heat engines are one in which the working medium is simultaneously coupled to a hot and cold bath at all times, while its Hamiltonian is continuously modulated[3][4][5]. Such heat engines have been studied using two-level system working mediums, as well as non-interacting multi-spin working mediums, in which the spins are collectively coupled to the hot and the cold bath[6][7]. Optimization of the many-body quantum heat engine using quantum control technique can be expected to take long time owing to the large dimension of the corresponding Hilbert space.

So we first optimize the performance of the continuous quantum heat engine(QHE) whose working medium (TLS) is periodically modulated by an external periodic pulse. The cost function that is to be optimized is the power output of the engine. The power output of the engine depends on the shape of the periodic pulse when we fix the parameter like the bath temperature, bare transition frequency of the TLS and modulation time period. Using CRAB we find a best possible shape of the periodic pulse which would maximize the power of the engine. Then we study the possibility of improving the performance of the multi-spin heat engine by using the optimal pulse obtained in case of a single spin heat engine. We show that using the optimal pulse of the single spin heat engine the performance of the many-body heat engine improves significantly.

This thesis report is organised as follows : In chapter 2, a detail quantum thermodynamical description of a quantum thermal engine and the laws of thermodynamics in quantum regime has been discussed as the preliminaries that are required to understand my thesis work. We have described thermodynamics of the continuous heat engine and how to deal with the dynamics of the reduced density matrix in the presence of the periodic modulation i.e the Floquet approach to the GKLS master equation. Chapter-3 contains the description of single spin continuous heat engine. The power and heat current expression for the sinusoidal modulation has been given. Then we optimized the power of the single spin heat engine using CRAB. Chapter-4 describes the collective heat engine where N spin-1/2 atoms are collectively interacting with the bath. We have analysed the collective effect which comes from the fact that the atoms are indistinguishable to the bath. We have also considered the sinusoidal modulation as an example of the periodic modulation for multi-spin heat engine as well. The conclusion and further question related to this thesis work has been described in chapter-4.

I am happy to share the news that the extension of this project is funded by the Chanakya fellowship sponsored by I-HUB quantum foundation, IISER Pune.

Chapter 2

Preliminaries

2.1 Quantum Thermal Machine

The thermodynamical description of the quantum thermal engine needs a well defined definition of the **heat and work** in quantum regime.

The energy of the system can be changed by two ways 1) Unitary way :By changing the Hamiltonian keeping the density matrix unchanged. 2) Non-unitary way: By Changing the system density matrix keeping the Hamiltonian unchanged. In first process the entropy of the system does not change by the definition of the unitary dynamics, the energy change corresponding to the first process is identified as work. In second case, the entropy changes because of the non unitary dynamics. Hence the energy change corresponding to the non unitary dynamics is called as heat in quantum regime. Unless bath and system are in an entangled state the above definition of the heat and work is valid for the all system coupled to thermal bath and undergoing Markovian dynamics.[8][9]

Mathematically the definition of the heat and work is given as ,

$$E = Tr[\rho H] \implies \Delta E = Tr[\rho(\Delta H)] + Tr[(\Delta\rho)H] \tag{2.1}$$

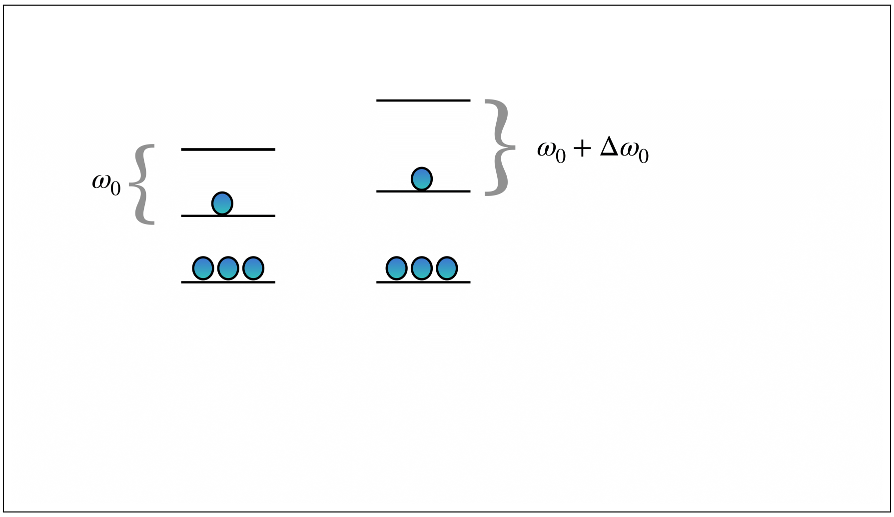

Figure 2.1: Increase energy by increasing the energy gap through Hamiltonian. ρ remains constant.$H = \hbar\omega_0 \sum_n |n\rangle\langle n| \rightarrow H = \hbar(\omega_0 + \Delta\omega_0)$

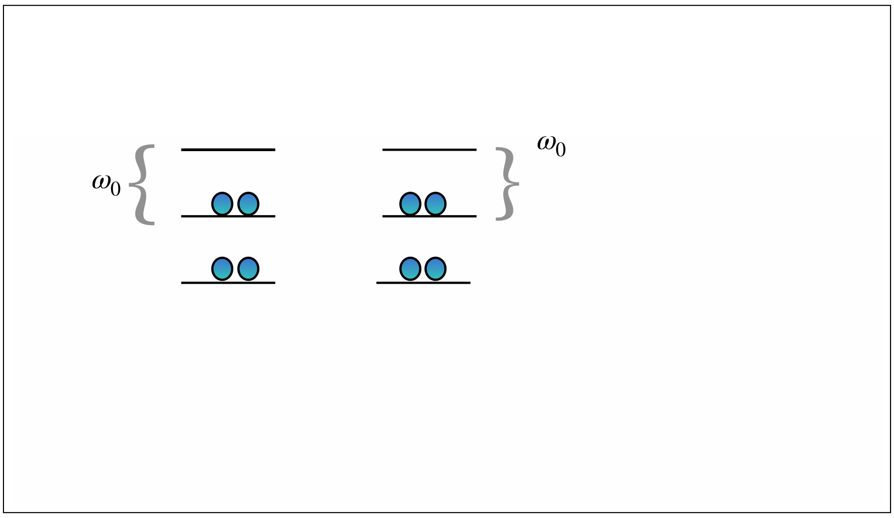

Figure 2.2: We increase energy by changing the state ρ of the system keeping the Hamiltonan fixed.Entropy changes because the state ρ is changing.This energy change is called Heat.

in equation 2.1 the term $Tr[\rho(\Delta H)]$ is identified as work while the second term $Tr[(\Delta\rho)H]$ is defined as heat.

2.1.1 Heat in quantum thermodynamics

The density matrix of the system is defined as follows [11] :

$$\rho = \sum_n p_n |n\rangle\langle n| \tag{2.2}$$

[0]The reference for the above part is R Alicki 1979 J. Phys. A: Math. Gen. 12 L103. [8]and [10]

and suppose we consider the Hamiltonian for the harmonic oscillator as,

$$H = \hbar\omega_0 \sum_n |n\rangle\langle n| \tag{2.3}$$

Then heat is given by,

$$Q_Q = Tr[\Delta\rho H] = \sum_n \Delta P_n E_n \tag{2.4}$$

the same expression for the heat can be derived from the Von-Neuman entropy relation[12]. We know that,

$$\begin{aligned} Q_s = T\Delta S &= T \cdot \Delta \left(-K_B \sum_n P_n \ln P_n \right) \\ &= -K_n T \sum_n (\Delta P_n) \ln p_n \end{aligned} \tag{2.5}$$

For the Gibbs state,we have

$$\begin{aligned} P_n &= \frac{e^{-E_n/K_B T}}{Z} \\ \Rightarrow Q_S &= -K_B T \sum_n (\Delta P_n) \ln P_n = \sum_n (\Delta P_n) E_n. \\ &= Q_Q. \end{aligned} \tag{2.6}$$

We observe that $Q_Q$and Q_S are same. So two definition of the heat matches with each other. Now as we know the heat and work in the quantum regime, we can discuss about the heat engines in quantum regime.

2.1.2 Quantum heat engines

A generic model of a microscopic quantum machine,similar to the classical thermal engine, consists of the following elements [4]

1. "Working Medium", which is a microscopic "small" quantum system $\mathcal{S}$.In clasical regime, generally the "working Medium" are gas molecules.In quantum regime, the working medium(WM) are quantum system. It could be a Two level system (TLS) or harmonoic oscillator or could be a many body quantum system.

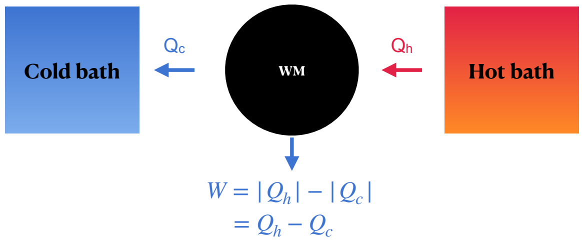

Figure 2.3: A schematic diagram of a quantum continuous heat engine

2. Cold and hot heat baths modelled by essentially infinite quantum systems at thermal equilibrium states.

3. External periodic driving.

In quantum heat engine the heat (J_h) flow from the hot bath to the system and part of it flows to the cold bath (J_c) any rest we get as power output. The model for microscopic engine can be realised as a model of quantum open system with a periodic Hamiltonian weakly coupled to heat baths.The weak coupling limit is important for the derivation of the dynamics of the system. The thermodynamical description of the model needs to identify the basic quantities like the internal energy E of $\mathcal{S}$, the entropy S of $\mathcal{S}$. the heat currents J_c, J_h entering $\mathcal{S}$ from the cold and hot bath, respectively, and the power P provided by external periodic forces. The Second Law of Thermodynamics for open system gives the inequality[13][10]

$$\frac{dS}{dt} - \frac{J_c}{T_c} - \frac{J_h}{T_h} \geq 0 \tag{2.7}$$

where T_c and T_h are temperatures of cold and hot bath, respectively. In (2.7) J_c/T_c, J_h/T_h are entropy flows from the baths and the (2.7) speaks about the positive entropy production. In the steady state regime (the state at which the density matrix remains constant respect to time). the average entropy $\bar{S}$ and the average energy $\bar{E}$ (averaged over a cycle) are constant. So the averaged heat currents and power satisfy the first law of thermodynamics,

$$\bar{J}_c + \bar{J}_h + \bar{P} = 0 \tag{2.8}$$

and the second law (2,7)

$$\frac{\bar{J}_c}{T_c} + \frac{\bar{J}_h}{T_h} \leq 0 \tag{2.9}$$

The machine operates as an engine if

$$\bar{J}_c < 0, \quad \bar{P} < 0,$$

The sign convention we follow here is that if the energy current leaves the system then it is negative. If it enters the system then it is positive. Then (2.8), (2.9) imply that the efficiency η satisfies the Carnot bound following by the 2nd law of thermodynamics,

$$\eta \equiv \frac{-\bar{P}}{\bar{J}_h} \leq \frac{T_h - T_c}{T_h} \tag{2.10}$$

In the refrigerator (heat pump) regime

$$\bar{J}_c > 0, \quad \bar{P} > 0, \tag{2.11}$$

which means that hot heat is extracted from a cold bath (cooling process) at the expense of positive work $\bar{P}$ supplied by the external driving. The coefficient of performance There are 2 different types of engines that are widely used in quantum thermodynamics (1) stroke engine (2) continuous engine. There are also other engine like szillard engine where the work is extracted from the information.

2.1.3 Stroke engine :

Stroke engines are also used in classical thermodynamics. Basically this engine operates in stroke . Here we give a brief description of the stroke engine because my project is related to the continuous engine. So we do not need anything about stroke engine. We explain the working principle of a stroke engine by an example: [14][15] **Otto cycle.** Otto cycle works in several stroke. We have discussed briefly about each strokes below :

1. Stroke-1 : We first start with the working medium(WM) in thermal equilibrium with the cold bath at temperature Tc. Then we change our WM Hamiltonian from $H(\nu_c)$ to the $H(\nu_h)$. The work done we get by this process is E_1(say). Notice that as we are changing the Hamiltonian the energy change is called work. ν_c and ν_h are the resonance frequency of the cold and hot bath.and the unitary dynamics is followed.

2. Stroke-2 : In second stroke we change WM state such that it get couple to the hot bath keepig the Hamiltonian constant. So it is an non unitary stroke. Heat Q_2 absorbs the system from the hot bath and finally the WM comes to the thermal equilibrium with the hot bath at Th.

3. Stroke-3: Wm medium is decoupled from the hot bath.The Hamiltonian changes from the H_h to H_c. The work done by the system is E_3(say).

4. Stroke-4 : We couple the W.M with the cold bath again and wait for the long time to reach at the thermal equilibrium state with the cold bath.(we reach the same initial state from where we stated). So according to the first law,

$$Q_1 + Q_2 + E_1 + E_3 = 0 \tag{2.12}$$

2.1.4 Continuous engine:

In microscopic engine the coupling and decoupling between bath and WM might be highly non trivial and might cost energy. So there is another type of engine called continuous engine where we do not need to couple and decouple again and again. The continuous engine are the one in which the working medium is simultaneously coupled to both the baths at all times while its Hamiltonian is periodically modulated by some external periodic modulation.[4][16][7]

In this case, the heat is continuously flowing from the hot bath to the system(Q_h) and from system to cold bath (Q_c). According to the first law of thermodynamics, the work out put of the engine is the difference between two heat current,$W = |J_h| - |J_c|$. Without periodic modulation, the working medium coupled to hat bath and cold bath, will eventually come into a thermal equilibrium state at a temperature in between hot bath and cold bath. So work output is zero. In order to get the work output, we need to take the system into a non equilibrium steady state by doing periodic modulation of the working medium[9]. The Hamiltonian of the total set up is :

$$H = H_s + H_{Bc} + H_{Bh} + \lambda_c H_{Ic} + \lambda_h H_{Ih}. \tag{2.13}$$

Here,H_s is time dependent because of the periodic modulation,

$$H_s(t) = H_s(t+\tau), \tau = \frac{2\pi}{\Delta} \tag{2.14}$$

where τ and Δ is the period and frequency of the modulation respectively. $H_B j$ for j=h,c are the bath Hamiltonian and $H_I j$ are the interaction Hamiltonian. The periodic modulation can be thought as the movement of piston in classical engine[7][4]. Before we discuss detail thermodynamics of the continuous engine we need to be familiar with how to deal the periodic modulation in the presence of the thermal bath. Generally we use Floquet approach to the Lindblad master equation for the periodic Hamiltonian.[9]

Floquet Expansion of GKLS master equation:

Floquet theory applies to the linear differential equations whose coefficients are the time periodic[17][18][4][7][19]. So here the Hamiltonian is periodic in time so the evolution of the reduced density matrix of the system contains the coefficient which are time periodic so we can apply Floquet theorem.

The Hamiltonian is periodically modulated as, $H_s(t) = H_s(t+\tau)$. Time evolution operator given as,

$$U(t,0) = \mathcal{T} \exp\left[-\frac{i}{t}\int_0^t H_s\left(t'\right) dt'\right] \tag{2.15}$$

Floquet theorem says that the time evaluation operator can be written as [4][7][9]

$$U(t,0) = P(t)e^{Rt} \tag{2.16}$$

where $P(t+\tau) = P(t)$ and operator R is a constant operator, at time t=0 we have

$$U(0,0) = \mathbb{I} \rightarrow \text{ identity operator } = P(0)$$

Since P is also periodic in time , So at any integer multiple of the period τ, P is an identity operator. So

$$P(n\tau) = I \text{ for } n = 0, 1, 2, \cdots$$

Finally we have the simplified version of the evolution operator as,

$$U(\tau, 0) = P(\tau)e^{R\tau} = e^{R\tau} \tag{2.17}$$

The operator R is related to the course gained Hamiltonian of the system which is time independent.We can always relate the operator R to the effective Hamiltonian stroboscopically[1]

$$U(\tau, 0) = e^{R\tau} = e^{-iH_{eff}\tau/h} \tag{2.18}$$

For example, consider a two level system whose Hamiltonian is $H(t) = \sigma_z\omega(t)$ and $H(t) = H(t + \tau)$ so U(τ, 0)=$\tau e^{-\frac{i}{\hbar\tau}}\sigma_z \int_0^\tau \omega\left(t'\right) dt'$ So we can see $H_{eff} = \sigma_z \frac{1}{\tau} \int_0^\tau \omega\left(t'\right) dt' = \bar{\omega}\sigma_z$ So The constant operator $R = \frac{-i}{\hbar}\bar{\omega}\sigma_z$.

The spectral decomposition of the effective Hamiltonian can be written in $|k\rangle$ basis as

$$H_{eff} = \sum_k \hbar\omega_k |k\rangle\langle k| \tag{2.19}$$

Where $\hbar k$ are the quasi energy. So,

$$e^{-i}H_{eff}t/h = \sum_k e^{-i\omega_k t} \mid k > \langle k| \tag{2.20}$$

Since P(t) is time periodic, we write its Fourier series expansion as

$$P(t) = \sum_q \tilde{P}(q)e^{-\lambda q\Delta t} \tag{2.21}$$

where q are the different Fourier mode and $\Delta = \frac{2\pi}{\tau}$ is the frequency of the modulation. $P(\nu)$ are the amplitude of the q'th Fourier mode.

$$\tilde{P}(\nu) = \frac{1}{\tau}\int_0^\tau P(t)e^{iv\Delta t}dt \tag{2.22}$$

1

[1]Stroboscopically means we are only looking into discrete time interval. Particularly at the end of the period.

Note that in case of the time independent working medium the q value are always zero and P(t) is always identity.

Master Equation

We are interested in the dynamics of the reduced density matrix of the system couple to the environments. For the simplicity let us consider only single Bath is coupled to the system. The Hamiltonian has the form

$$H = H_S(t) + H_B + \lambda S \otimes B \tag{2.23}$$

In interaction picture S(t) is given as,

$$S(t) = U^{+}(t,0) S \cup (t,0) = \sum_{q} \sum_{\{\omega'_j\}} S_{q\omega} e^{-i(\omega+q\Delta)t} \tag{2.24}$$

In the right side of the above equation the term qΔ comes from the P(t) (Since the propagator (2.13) U contains P(t) as well as R,) and the term ω is the energy gap of the system which comes from the constant operator R. When the Hamiltonian is time independent, in interaction picture, the system operator has the form

$$S(t) = \sum_{\omega'_j} S_{\omega} e^{-i(\omega)t} \tag{2.25}$$

So in case of the periodic modulation we have additional Fourier mode term in contrast to the time independent Hamiltonian. Once we have the equation(2.24) we can immediately write the master equation by following the same analogy that has been done for the constant hamiltonian. We assume the following assumption for the validity of the GKLS equation.

1. Weak coupling limit : The working medium is weakly coupled to the thermal Bath. Weak coupling limit leads to 2nd order perturbation problem.

2. Born and Markov Approximation : The bath size is very large compare to the system size, so in weak coupling limit, we assume that the bath state does not change with respect to time. In other words the bath changes so fast that it is apparently remains constant withe respect to the system thermalization time. . Markov approximation depend on the fact that the dynamics of the system does not depend on its past history.

3. In order to make a thermodynamic consistent theory We consider the global approach to the master equation[[20]]. In other words we perform the secular approximation by dropping the fast oscillatory term from the Master equations.

The master equation at steady state reads as [2]

$$\dot{\rho}(t) = \mathcal{L}\left[\rho_s(t)\right] \tag{2.26}$$

the subliovian is given by,

$$\mathcal{L} = \sum_q \sum_{\{\omega\}} \mathcal{L}_{\omega,q}\left[\rho_{ss}(t)\right] \tag{2.27}$$

Where,

$$\mathcal{L}_{q,\omega}\left[\rho_{ss}(t)\right] = \frac{1}{2}P(q)G(\omega_0 + q\Delta)\left[2S_{q,\omega}\rho_s S^+_{q,\omega} - \rho_s S^+_{q,\omega}S_{q,\omega} - S^+_{q,\omega}S_{q,\omega}\rho_s\right] \tag{2.28}$$

where, P(q) represents the weights of the qth floquet mode. P(q) is given by,

$$P(q) = |\xi(q)|^2$$

where,

$$\xi(q) = \frac{1}{\tau}\int_0^\tau \exp\left(i\int_0^t \left(\omega(s) - \omega_0\right) ds\right) e^{-iq\Delta t} dt$$

Using the KMS condition i.e the global detail balance condition, where β is the inverse efective temperature. we can write,

$$G(-\omega_0 - q\Delta) = e^{-(\omega_0 + q\Delta)\beta} G(\omega_0 + q\Delta) \tag{2.29}$$

the Fourier components also appears in the bath spectral function implies that the coupling also depends the q'th energy side-band.By dropping the negative ω we can write the Lindblad superoperator as as,

$$\mathcal{L} = \sum_{\boldsymbol{q}} \sum_{\{\omega>0\}} \mathcal{L}_{q,\omega} \tag{2.30}$$

[2]1

[2]The reference for the above part is [9][21][4]

And the final master equation reads as

$$\begin{aligned}\mathcal{L}_{q,\omega}[\rho_s] = \frac{1}{2}G(\omega_0+q\Delta)P(q)\left(2S_{q,\omega}\rho_{ss}S^{+}_{q,\omega} - S^{+}_{q,\omega}S_{q,\omega}\rho_s - \rho_s S^{+}_{q,\omega}S_{q,\omega}\right) \\ +\frac{1}{2}e^{-\beta\hbar(\omega+q\Delta)}G(\omega+q\Delta)P(q)\times\left[2S^{+}_{q,\omega}\rho_s S_{q,\omega} - S_{q,\omega}S^{+}_{q,\omega}t_0 - \rho_s S_{q,\omega}S^{+}_{q,\omega}\right]\end{aligned} \tag{2.31}$$

each subliovilian gives rise to the Gibbs like state,

$$\tilde{\rho}_{q,\omega} = Z^{-1}\exp\left[-\beta\frac{(\omega+q\Delta)}{\omega}H_{eff}\right] \tag{2.32}$$

For multiple baths $j = h, c$

$$\mathcal{L} = \sum_q\sum_\omega\sum_j \mathcal{L}_{j,q,\omega} \tag{2.33}$$

$G(\omega_0+q\Delta) \rightarrow G_j(\omega+q\Omega)$ and $S_{q,\omega} \rightarrow S_{j,q,\omega;}$; $\quad \beta \rightarrow \beta_j$

Heat, Work, and the laws of thermodynamics of the continuous engine.

In equation(2.1) we have seen the defination of the heat and work in quantum regime. In order to define the heat the heat flow in a continuous engine operation let us define the relative entropy which is some how related to distance between two state.[22][23]

$$S\left(\rho\|\rho'\right) = k_b Tr\left[\rho\left(\ln\rho - \ln\rho'\right)\right] \tag{2.34}$$

We can show that the relative entropy S is always greater than equal to zero. It is zero only when $\rho = \rho\prime$ that is two state are same. In information theory the relative entropy has the exact same form without any k_b. Here the k_b relates to the thermodynamics.

We know that in Markovian dynamics, the distance between initial states and final states (steady state ρ_{ss}) always decreases monotonically in time [9][10][24]. So in the regime of the Markov approximation The time derivative of the relative entropy is always less than equal to zero.This is called Sphons in equality[22].

$$\frac{d}{dt}S\left(\rho\|\rho_{ss}\right) \leq 0 \tag{2.35}$$

equation [2.34] leads to the following expression :

$$\frac{d}{dt}k_B T_r \left[\rho \ln \rho - \rho \ln \rho_{ss}\right] \leq 0 \tag{2.36}$$

But we know that the Von-Newman entorpy is[12]

$$S_{vn} = k_b T_r \left[\rho \ln \rho\right] \tag{2.37}$$

So the first term in the left part of the inequality[2.36] can be identified as

$$k_B \frac{d}{dt} \operatorname{Tr}(\rho \ln \rho) = -\frac{dS_{vn}}{dt} \tag{2.38}$$

and the second term of the inequality can be expanded as follows

$$k_B \frac{d}{dt} T_r \left[\rho \ln \rho_{ss}\right] = k_B \operatorname{Tr}_r \left[\dot{\rho} \ln \left(\frac{e^{-\beta H}}{z}\right)\right] = -\frac{\operatorname{Tr}[\dot{\rho} H]}{T} = -\frac{1}{T}\frac{d\varphi}{dt} \tag{2.39}$$

The terms which are proportional to the $T_r(\dot{\rho})$ in equation[] vanishes because the ρ being the density matrix the diagonal term gives the probability and the sum of the probability is one so derivative of it is zero. The left side of the above equation is the rate of change of the heat. So finally we have the in equality,

$$\frac{dS_{vn}}{dt} - \frac{1}{T}\frac{d\varphi}{dt} \geq 0 \tag{2.40}$$

which is nothing but the second law of thermodynamics. The system is coupled to the bath, the change in entropy of the system is change in the Von-Newman entropy and the entropy change due to the baths is $\frac{1}{T}\frac{d\varphi}{dt}$ So the global change in entropy is always greater than zero. Other way of looking into the 2nd law of thermodynamics is the Sphons inequality.

$$\frac{d}{dt} S\left(\rho \| \rho_{ss}\right) \leq 0 \tag{2.41}$$

As we know the equilibrium state has maximum entropy so the systems is always going towards the maximum entropy state.

Here we have used the Markovian dynamics but in any case it is valid for the Non Markovian dynamics as well.

In continuous heat engine the heat current and work are important.The heat current $J_j = \frac{d\varphi_j}{dt}$. We replace $\dot{\rho}$ in Lindbladian form and the steady state solution in place ρ_{ss} in inequality in 2.42,

$$\frac{d}{dt}S_{vn}(\rho(t)) + k_B T_r \sum_{q,\omega,j} T_r \left[\mathcal{L}^j_{\omega,q}(\rho(t)) \ln \tilde{\rho}_{\omega,q}\right] \geq 0 \tag{2.42}$$

But we know that,

$$\frac{d}{dt}S_{vn}(\rho(t)) - \sum_j \frac{1}{T_j}\frac{d\varphi_j}{dt} \geq 0 \tag{2.43}$$

In terms of the heat current we write as ,

$$\frac{d}{dt}S_{vn}(\rho(t)) - \sum_j \frac{J_j}{T_{j'}} \geq 0 \tag{2.44}$$

Now comparing the above two in equality we can identify the heat current as

$$J_j(t) = -k_B T_j \sum_{q,\{\omega \geq 0\}} T_r \left[\mathcal{L}^j_{\omega,q}(\rho(t)) \ln \tilde{\rho}^j_{\omega,q}\right] \tag{2.45}$$

For the non equilibrium steady state the heat current can be expressed as

$$J_j(t) = \sum_{q,\{\omega \geq 0\}} \frac{\omega + q\delta}{\omega} T_r \left[\mathcal{L}^j_{\omega,q}\left(\rho_{ss}\right) H_{eff}\right] \tag{2.46}$$

The first law in continuous engine gives

$$\sum_j J_j = P \tag{2.47}$$

where the P is the power output of the engine.

Chapter 3

Single spin quantum continuous heat engine

3.0.1 Introduction

A two-level system(TLS) continuous engine can be described as follows: a two level system working medium(WM)is simultaneously coupled to a hot and a cold bath. The Hamiltonian of the total set up can be written as (figure 3.1)[8][7]

$$H = H_0 + H_{Bc} + H_{Bh} + H_{Ic} + H_{Ih} \tag{3.1}$$

Here,

$$H_0 = \omega(t)\sigma^z \tag{3.2}$$

is the Hamiltonian of the TLS.

$$H_B = H_{Bc} + H_{Bh} \tag{3.3}$$

is the bath Hamiltonian and,

We consider periodic modulation of the TLS, such that $\omega(t+\tau) = \omega(t)$, where τ is the modulation period. The WM-bath interaction Hamiltonian is given by

$$H_{Ij} = \lambda_j \sigma^x \otimes B_j \tag{3.4}$$

where B_j is the bath operator and $j = h, c$ refers to the hot or the cold bath, respectively.

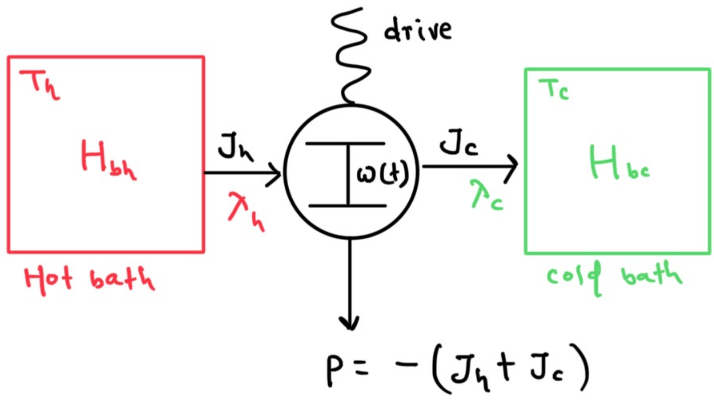

Figure 3.1: A schematic diagram of a single spin quantum continuous heat engine modelled by a two level system WM. The heat flows from hot bath(Jh) to the system, part of it (Jc) goes to the cold bath and rest (P) we get as work output.

The coupling strength is $0 < \lambda_j \ll 1$.The weak coupling limit is ensured by the small value of the $_j$ The heat bath can be realised as the fermionic or bosonic gas described by second quantization formalism in thermodynamic limit [9]. For a Bosonic bath the bath operator B_j , can be chosen as the combination of the annhilation and creation operator describing the emission and absorption of the photon or phonon While for the fermionic bath, observable has the bilinear form of the annhileation and creation operator. But to derive fundamental master equation of the reduced system,we do not need the exact detail of the interaction Hamiltonian and the bath. we only need the bath correlation function.

3.0.2 Markovian Master Equation.

We are interested in the dynamics of the reduced density matrix $\rho(t)$ of the TLS. The $\rho(t)$ can be given as,

$$\rho(t) = \mathrm{Tr}_B \left(U_{\mathrm{tot}}(t) \rho \otimes \rho_B U_{\mathrm{tot}}(t)^\dagger \right), \tag{3.5}$$

Where the $U(t)$ is the time evolution operator of the total system satisfying the following equation

$$\frac{d}{dt} U_{\mathrm{tot}}(t) = -i \left(H_0(t) + H_{\mathrm{int}} + H_B \right) U_{\mathrm{tot}}(t) \tag{3.6}$$

The initial state(3.5) is assumed to be a direct product state and bath state ρ_B is time independent which implies the weak coupling assumption and the Born approximation[ref-2]. Bath state are product of the two thermal equilibrium state at a temperature T_j.

$$\rho_B = \rho_B^{(c)} \otimes \rho_B^{(h)}, \quad \rho_B^{(j)} = \frac{e^{-H_B^{(j)}/T_j}}{\mathrm{Tr}\left(e^{-H_B^{(j)}/T_j}\right)}, \quad j = c, h. \tag{3.7}$$

Here,in equation(1) Tr_B means the taking partial trace of the total system with respect to the environmental degree of freedom. We want a simpler form of approximate equation of motion for $\rho(t)$ which is thermodynamcally consistent. Here we use the Markovian dynamics of the reduced density matrix of the TLS. The state ρ of the WM evolves following the master equation in the Schrodinger picture is given by [8][4][7]

$$\dot{\rho} = -i[H(t), \rho(t)] + \sum_{j,q} P_q \mathcal{L}_{j,q}[\rho], \tag{3.8}$$

where $\mathcal{L}_{j,q}$ denotes the Lindblad super operator corresponding to the j-th bath. The exact form of the Linblad superoperator depends on the structer of the interaction Hamiltonian**??** in the interaction picture.

$$H_{\text{int}}(t) = \sigma^x(t) \otimes \left(B^c(t) + B^h(t)\right) \tag{3.9}$$

Where,

$$\sigma^x(t) = \exp\left(\frac{i}{2}\int_0^t \omega(s)\sigma^z ds\right)\sigma^x \exp\left(-\frac{i}{2}\int_0^t \omega(s)\sigma^z ds\right) \tag{3.10}$$

and,

$$B^j(t) = e^{iH_R^{(j)}t} B^j e^{-iH_B^{(j)}t} \tag{3.11}$$

The Fourier decomposition of the $\sigma_x(t)$ in presence of the perioic modulation given by [9][4][17][7],

$$\sigma^x(t) = \sum_{q\in\mathbb{Z}} \left(\xi(q)e^{-i(\omega_0+q\Omega)t}\sigma^- + \bar{\xi}(q)e^{i(\omega_0+q\Omega)t}\sigma^+\right) \tag{3.12}$$

Where,

$$\xi(q) = \frac{1}{\tau}\int_0^\tau \exp\left(i\int_0^t (\omega(s) - \omega_0)\, ds\right) e^{-iq\Omega t} dt \tag{3.13}$$

follows the Fourier series properties,

$$\sum_{q\in Z} |\xi(q)|^2 = 1 \tag{3.14}$$

In equation (3.12) the term $\xi_q\sigma^-$($\xi_q\sigma^+$) represent the de-excitation (excitation) of the effective Hamiltonian $\bar{H} = \frac{1}{2}\bar{\omega}\sigma_z$ with the probability amplitude of the $\xi(q)$ which depends on the shape of the modulation.The oscillating term in equation(12) represents that the bath exchange energy at the frequency $\omega_0 + q\Omega$ with the periodically driven two level system. the ω_0 terms comes from the bare Hamiltonian of the working medium while $q\Omega$ terms comes from the external source of the modulation. Total probability rate of the two process is given by the product of

$$P(q) = |\xi(q)|^2 = P(-q) \tag{3.15}$$

and the bath spectral function at the frequency, $\omega_0 + q\Omega$.The form of the bath spectral function is given by

$$G^j(\omega) = \int_{-\infty}^{+\infty} e^{i\omega t}\, \mathrm{Tr}\left(\rho_B^j B^j(t) B^{a=j}\right) dt \tag{3.16}$$

The KMS(Kubbo-Martin -Scwinger) condition ,

$$G^j(-\omega) = e^{-\omega/T_j} G^j(\omega), \tag{3.17}$$

characterize the thermal equilibrium state. So combining above information we can write the form of the Lindblad super operator for our system in terms of the jump operator σ^+ and σ^- as,

$$\mathcal{L} = \mathcal{L}^c + \mathcal{L}^h, \quad \mathcal{L}^j\rho = \sum_{q\in\mathbb{Z}} \mathcal{L}_q^j \rho \tag{3.18}$$

Where, the Subliovilian given as,

$$\begin{aligned} \mathcal{L}_q^j\rho = &\frac{P(q)}{2}\left\{G^j(\omega_0 + q\Omega)\left(\left[\sigma^-\rho, \sigma^+\right] + \left[\sigma^-, \rho\sigma^+\right]\right)\right. \\ &\left. + G^j(-\omega_0 - q\Omega)\left(\left[\sigma^+\rho, \sigma^-\right] + \left[\sigma^+, \rho\sigma^-\right]\right)\right\} \end{aligned} \tag{3.19}$$

Here the $\mathcal{L}$ is time independent. but in general it is not the case, for the complicated Hamiltonian with non diagonal entries the superoperator is time dependent.[]. The jump operator do not mix the diagonal part to the non diagonal part in the master equation. they evolves independently in σ_z basis. and satisfy the Pauli master equation of the form ($p_k \equiv \rho_{kk}$)

$$\frac{dp_1}{dt} = \gamma_\downarrow p_2 - \gamma_\uparrow p_1, \quad p_1 + p_2 = 1. \tag{3.20}$$

The overall damping and pumping rates are given by sums of "local" ones

$$\gamma_\downarrow = \gamma_\downarrow^c + \gamma_\downarrow^h, \quad \gamma_\downarrow^j = \sum_{q\in\mathbb{Z}} \gamma_\downarrow^j(q), \quad \gamma_\downarrow^j(q) = P(q) G^j(\omega_0 + q\Omega), \tag{3.21}$$

$$\gamma_\uparrow = \gamma_\uparrow^c + \gamma_\uparrow^h, \quad \gamma_\uparrow^a = \sum_{q\in\mathbb{Z}} \gamma_\uparrow^a(q), \quad \gamma_\uparrow^a(q) = P(q)G^a\left(-\omega_0 - q\Omega\right) \tag{3.22}$$

The relation (27) implies "local" detailed balance

$$\gamma_\uparrow^a(q) = e^{-(\omega_0+q\Omega)/T_a}\gamma_\downarrow^a(q). \tag{3.23}$$

Notice the additivity of damping and pumping rates with respect to different baths and different harmonics of the driving force.

One can easily show that the off-diagonal elements of the density matrix tend to zero, and hence the system possesses a stationary Gibbs state given as,

$$\rho_{ss} = \text{diag}\left[\frac{\gamma_\downarrow}{\gamma_\downarrow + \gamma_\uparrow}, \frac{\gamma_\uparrow}{\gamma_\downarrow + \gamma_\uparrow}\right].$$

(3.24)

Finally, we recall Spohn inequality valid for any LGKS superoperator $\mathcal{L}$ with a stationary state ρ_{ss} (i.e. $\mathcal{L}\rho_{ss} = 0$)

$$\text{Tr}[\mathcal{L}\rho(\ln\rho - \ln\rho_{ss})] \leq 0 \tag{3.25}$$

and the $q = 0, \pm1, \pm2, \ldots -$ th Floquet mode, with weight $0 \leq P_q \leq 1$ and frequency $\omega_q = \omega_0 + q\Omega$. Usually P_q is small for large q, so that it is enough to consider finite number of Floquet mode.

3.0.3 Heat Current, Work and the laws of thermodynamics.

Environment exchanges both energy and entropy with the coupled working medium. So heat current must be determined from the dissipiative part of the master equation given by the Lindblad super operator. The heat current is given by,

$$J(t) = J_c(t) + J_h(t), \quad J_j(t) = \sum_{q\in\mathbb{Z}} J_j^q(t). \tag{3.26}$$

Here $J_j^q(t)$ is the heat currents entering to the TLS working medium from the bath at a given Floquet harmonics q. The local current $J_j^q(t)$ is the product of the probability flow from the ground state to the excited state of the averaged Hamiltonian and total energy quantum$(\omega_0+q\Omega)$ which contains energy provided by a given harmonic of external perturbation.

$$J_j^q(t) = \frac{1}{2}\left(\omega_0 + q\Omega\right)\mathrm{Tr}\left(\sigma^z \mathcal{L}_q^j \rho(t)\right) \tag{3.27}$$

Defining the entropy of the TLS state as the von Neumann entropy

$$S(t) = -\,\mathrm{Tr}(\rho(t)\ln\rho(t)) \tag{3.28}$$

one can show that the II-law in the form (2) is satisfied. To prove it we use the identity valid for any Markovian master equation with a dissipative part given by $\mathcal{L}$,

$$\frac{dS(t)}{dt} = -\,\mathrm{Tr}[(\mathcal{L}\rho(t))\ln\rho(t)] \tag{3.29}$$

and the fact that any piece $\mathcal{L}_q^a$ of our generator is also a LGKS generator with its own stationary state of the Gibbs-like form

$$\tilde{\rho}_q^a = \frac{e^{-\frac{1}{2}(\omega_0+q\Omega)\sigma^3/T_a}}{\mathrm{Tr}\, e^{-\frac{1}{2}(\omega_0+q\Omega)\sigma^3/T_a}} \tag{3.30}$$

Then one can use the inequality (37) for any single pair $\left(\mathcal{L}_q^a, \tilde{\rho}_q^a\right)$ and combine it with (40) and the definition of current (38), (39) to obtain (2).

Heat currents at the stationary state $\tilde{\rho}$ can be defined as,

$$\bar{J}_j = \frac{1}{2}\sum_{q\in\mathbb{Z}}\left(\omega_0 + q\Omega\right)\mathrm{Tr}\left(\sigma^z \mathcal{L}_q^a \tilde{\rho}\right), \quad j = c, h \tag{3.31}$$

Now we can have the explicit form of the heat current for periodically modulated TLS WM by putting the steady state solution and the matrix form of the σ_+, σ_- operator. The J_j is given by,

$$J_{C(H)} = \sum_m \left(\omega_0 + m\Delta\right) P_m G^{c(h)}\left(\omega_0 + m\Delta\right)\frac{e^{-\frac{(\omega_0+m\Delta)}{T_{c(h)}}} - w}{w+1} \tag{3.32}$$

Where,the population ration w at steady state is given by

$$w = \frac{\tilde{\rho_{ee}}}{\tilde{\rho_{gg}}} = \frac{\sum_{q,j} P_m G^j \left(\omega_0 + m\Delta\right) e^{-\frac{\omega_0 + m\Delta}{T_j}}}{\sum_{m,j} P_m G^j \left(\omega_0 + m\Delta\right)} \tag{3.33}$$

The I-law can now be used to define the stationary power $\bar{P}$ as in (3)

$$\bar{P} = -\bar{J}_c - \bar{J}_h \tag{3.34}$$

Using the equation (78) we can find the power expression as

$$\mathcal{P} = \sum_{m,j} \frac{\left(\omega_0 + m\Delta\right) P_m}{w+1} \left[G^j \left(\omega_0 + m\Delta\right) \left(w - e^{-\frac{\left(\omega_0 + m\Delta\right)}{T_j}} \right) \right] \tag{3.35}$$

Remark-1 : In contrast to models with slowly varying external forces studied in [16], the definition of work and internal energy, independent of the I-law, is an open problem for the case of arbitrary modulation. Therefore, only in the case of stationary regime we have the unambiguous definition of average power.

3.0.4 Universal Machine operation Mode

The engine can either act as a heat engine (or a refrigerator) depending on the direction of the heat flow from the environment to the working medium (or working medium to the environment). The sign convention we follow is that if the energy current enters the system then it is positive and if the energy current leaves the system then it is negative.So the heat engine regime is defined as the heat current J_h is positive because it flows from the bath to the system and the cold current J_c, and power output P are negative. The J_h is negative and J_c, P are positive in the refrigerator regime. Mainly, the following parameters decides the direction of the current flow in the operation of quantum machine.[7][4][16]

1. Choice of the bath spectral function
2. Shape of the modulation $\omega(t)$.

In the following example we would see how the choice of the bath spectral function helps in the coupling and decoupling of the system with bath at different cut of frequency which allow us to have a non equilibrium steady state with non zero power output. The shape of the driving pulse plays an important role in the performance of the quantum heat engine. In subsequent section we consider a sinusoidal pulse as an example of the periodic pulse and discuss its effect on the energy current.

An example : Sinusoidal Modulation

We consider a sinusoidal modulation of the form. The example of sinusoidal modulation has already been considered in

$$\omega(t) = w_0 + \lambda\Delta \sin(\Delta t), \tag{3.36}$$

With the condition,

$$0 \leq \lambda \leq 1 \tag{3.37}$$

Under the condition (3.37) we observe that only $q = 0, \pm 1$ harmonics contribute to the energy current.This can be seen if we put sinusoidal modulation form(3.36) in the expression of the $\xi(q)$ (3.13) The Floquet weitage of the these harmonics are,

$$P_{q=0} \simeq 1 - \frac{\lambda^2}{2}, \quad P_{q=\pm 1} \simeq \frac{\lambda^2}{4} \tag{3.38}$$

As the value of the λ is very small higher terms are significantly small. Generally the derivation of the heat current including all Floquet mode is very difficult (analytically). Here we have given the general expression of the heat current and power in the presence of the sinusoidal modulation

$$\begin{aligned}\mathcal{P} = &-\frac{\Delta}{\sum_{q,i=H,C} P_q G^j\left(\omega_0 + q\Delta\right)\left(1 + e^{-\frac{q_0+q\Delta}{T_i}}\right)} \Big\{ P_1 P_0 \Big[G^C\left(\omega_0+\Delta\right) G^C\left(\omega_0\right)\left(e^{-\frac{a_0+\Delta}{T_C}} - e^{-\frac{\omega_0}{T_C}}\right) \\
&+ G^C\left(\omega_0+\Delta\right) G^H\left(\omega_0\right)\left(e^{-\frac{\omega_0+\Delta}{T_C}} - e^{-\frac{u_0}{T_H}}\right) + G^H\left(\omega_0+\Delta\right) G^C\left(\omega_0\right)\left(e^{-\frac{\omega_0+\Delta}{T_H}} - e^{-\frac{q_0}{T_C}}\right) \\
&+ G^C\left(\omega_0-\Delta\right) G^C\left(\omega_0\right)\left(e^{-\frac{q_0}{T_C}} - e^{-\frac{\omega_0-\Delta}{T_C}}\right) + G^H\left(\omega_0-\Delta\right) G^C\left(\omega_0\right)\left(e^{-\frac{q_0}{T_C}} - e^{-\frac{\omega_0-\Delta}{T_H}}\right) \\
&+ G^C\left(\omega_0-\Delta\right) G^H\left(\omega_0\right)\left(e^{-\frac{\rho_0}{T_H}} - e^{-\frac{\omega_0-\Delta}{T_C}}\right) + G^H\left(\omega_0+\Delta\right) G^H\left(\omega_0\right)\left(e^{-\frac{\omega_0+\Delta}{T_H}} - e^{-\frac{q_0}{T_H}}\right) \\
&+G^H\left(\omega_0-\Delta\right) G^H\left(\omega_0\right)\left(e^{-\frac{e_0}{T_H}} - e^{-\frac{c_0-\Delta}{T_H}}\right)\Big] + 2P_1^2 \Big[G^C\left(\omega_0+\Delta\right) G^C\left(\omega_0-\Delta\right)\left(e^{-\frac{\omega_0+\Delta}{T_C}} - e^{-\frac{\omega_0-\Delta}{T_C}}\right) \\
&+ G^C\left(\omega_0+\Delta\right) G^H\left(\omega_0-\Delta\right)\left(e^{-\frac{a_0+\Delta}{T_C}} - e^{-\frac{q_0-\Delta}{T_H}}\right) + G^H\left(\omega_0+\Delta\right) G^C\left(\omega_0-\Delta\right)\left(e^{-\frac{q_0+\Delta}{T_H}} - e^{-\frac{\alpha_0-\Delta}{T_C}}\right) \\
&+G^H\left(\omega_0+\Delta\right) G^H\left(\omega_0-\Delta\right)\left(e^{-\frac{\omega_0+\Delta}{T_H}} - e^{-\frac{\omega_0-\Delta}{T_H}}\right)\Big]\Big\}.\end{aligned} \tag{3.39}$$

and the hot current is given by,

$$
\begin{aligned}
J_H =& \frac{1}{\sum_{m,i=H,C} P_m G^i\left(\omega_0+m\Delta\right)\left(1+e^{-\frac{\omega_0+m\Delta}{T_i}}\right)}\left\{P_0^2\omega_0 G^H\left(\omega_0\right)G^C\left(\omega_0\right)\left(e^{-\frac{\omega_0}{T_H}}-e^{-\frac{\omega_0}{T_C}}\right)\right.\\
&+P_1P_0\left[-\omega_0 G^C\left(\omega_0+\Delta\right)G^H\left(\omega_0\right)\left(e^{-\frac{\omega_0+\Delta}{T_C}}-e^{-\frac{\omega_0}{T_H}}\right)\right.\\
&+\left(\omega_0+\Delta\right)G^H\left(\omega_0+\Delta\right)G^C\left(\omega_0\right)\left(e^{-\frac{\omega_0+\Delta}{T_H}}-e^{-\frac{\omega_0}{T_C}}\right)\\
&-\left(\omega_0-\Delta\right)G^H\left(\omega_0-\Delta\right)G^C\left(\omega_0\right)\left(e^{-\frac{\omega_0}{T_C}}-e^{-\frac{\omega_0-\Delta}{T_H}}\right)+\omega_0 G^C\left(\omega_0-\Delta\right)G^H\left(\omega_0\right)\left(e^{-\frac{a_0}{T_H}}-e^{-\frac{a_0-\Delta}{T_C}}\right)\\
&\left.+\Delta G^H\left(\omega_0+\Delta\right)G^H\left(\omega_0\right)\left(e^{-\frac{\omega_0+\Delta}{T_H}}-e^{-\frac{\omega_0}{T_H}}\right)+\Delta G^H\left(\omega_0-\Delta\right)G^H\left(\omega_0\right)\left(e^{-\frac{a_0}{T_H}}-e^{-\frac{\omega_0-\Delta}{T_H}}\right)\right]\\
&+P_1^2\left[-\left(\omega_0-\Delta\right)G^C\left(\omega_0+\Delta\right)G^H\left(\omega_0-\Delta\right)\left(e^{-\frac{\omega_0+\Delta}{T_C}}-e^{-\frac{a_0-\Delta}{T_H}}\right)\right.\\
&+\left(\omega_0+\Delta\right)G^H\left(\omega_0+\Delta\right)G^C\left(\omega_0-\Delta\right)\left(e^{-\frac{\omega_0+\Delta}{T_H}}-e^{-\frac{a_0-\Delta}{T_C}}\right)\\
&+2\Delta G^H\left(\omega_0+\Delta\right)G^H\left(\omega_0-\Delta\right)\left(e^{-\frac{a_0+\Delta}{T_H}}-e^{-\frac{\omega_0-\Delta}{T_H}}\right)\\
&+\left(\omega_0-\Delta\right)G^H\left(\omega_0-\Delta\right)G^C\left(\omega_0-\Delta\right)\left(e^{-\frac{a_0-\Delta}{T_H}}-e^{-\frac{a_0-\Delta}{T_C}}\right)
\end{aligned}
\tag{3.40}
$$

The cold current can be derived from the above equation by changing the H to C. So as we can see the analytical expression for the energy currents are complicated it gets even more complicated when we include higher Floquet mode for the different shape of the modulation. and For the simplicity, we assume the following bath spectral function for the sinusoidal modulation,

$$
G^C(\omega)\simeq 0 \quad \text{for} \quad \omega\geq\omega_0, \quad G^H(\omega)\simeq 0 \quad \text{for} \quad \omega\leq\omega_0 \tag{3.41}
$$

Below frequency ω_0, hot bath do not share the energy with the working medium and above ω_0 the cold bath do not share the energy hence we would get a non zero power output. Having above cut off bath spectral function the power output and the energy current reduced to a simpler form,

$$
\begin{aligned}
J_H &= \left(\omega_0+\Delta\right)\mathcal{N}\left(e^{-\left(\frac{\omega_0+\Delta}{T_H}\right)}-e^{-\left(\frac{\omega_0-\Delta}{T_C}\right)}\right)\\
J_C &= -\left(\omega_0-\Delta\right)\mathcal{N}\left(e^{-\left(\frac{\omega_0+\Delta}{T_H}\right)}-e^{-\left(\frac{\omega_0-\Delta}{T_C}\right)}\right)\\
\mathcal{P} &= -2\Delta\mathcal{N}\left(e^{-\left(\frac{a_0+\Delta}{T_H}\right)}-e^{-\left(\frac{a_0-\Delta}{T_C}\right)}\right)
\end{aligned}
\tag{3.42}
$$

Where the constant N is given by,

$$
\mathcal{N}=\frac{\lambda^2}{4}\frac{G^C\left(\omega_0-\Delta\right)G^H\left(\omega_0+\Delta\right)}{G^C\left(\omega_0-\Delta\right)\left[1+e^{-\left(\frac{\omega_0-\Delta}{T_C}\right)}\right]+G^H\left(\omega_0+\Delta\right)\left[1+e^{-\left(\frac{e_0+\Delta}{T_H}\right)}\right]} \tag{3.43}
$$

We see that depending on the parameter Δ the sign of the heat current can change. There exist a critical delta Δ_{cr} for the sinusoidal modulation at which the power becomes zero. For $\Delta \geq \Delta_{cr}$ the heat engine works as a refrigerator. We can calculate the Δ_{cr} from equation (88) by observing the sign change. For the sinusoidal modulation, Δ_{cr} is given by,

$$\Delta_{cr} = \omega_0 \frac{Th - Tc}{Th + Tc}. \tag{3.44}$$

Below critical frequency of the modulation the engine act as heat engine with efficiency,

$$\eta = \frac{2\Delta}{\omega_0 + \Delta} \tag{3.45}$$

Above critical frequency , the engine act as the refrigerator with COP,

$$COP = \frac{\omega_0 - \Delta}{2\Delta} \tag{3.46}$$

At Δ=Δ_{cr}, The engine reaches its maximum Carnot efficiency correspondingly the power goes to zero. The operation mode changes to prevent from violating II-law of thermodynamics.

3.0.5 Plots for sinusoidal modulation

We have reproduced the power Vs Delta plot for the sinusoidal modulation. We show that there exist a critical Δ_{cr} at which the power goes to zero and the engine change its operation mode. That is the hot current Jh becomes negative and power becomes positive.

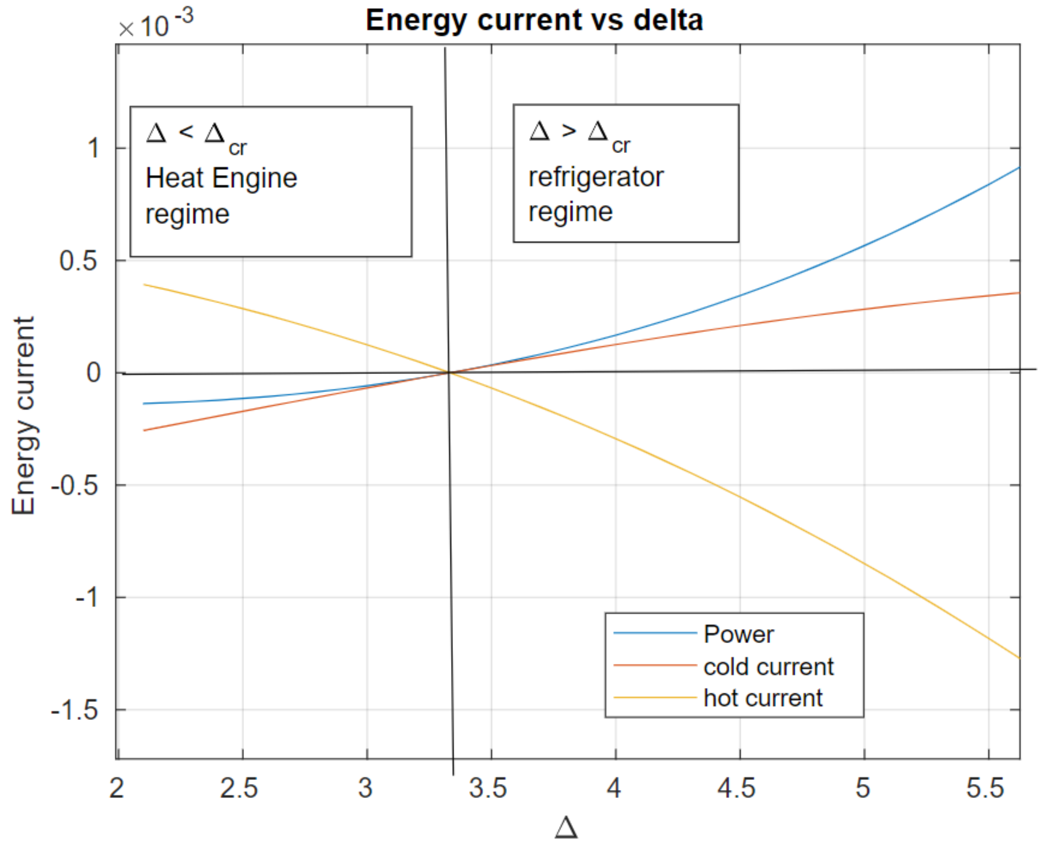

Figure 3.2: Energy current VS frequency of the sinusoidal modulation plot. The value of the Δ_{cr} is 3.39 $s-1$. Above the critcal delta engine operates as a refrigerator because $J_c > 0, J_h < 0, P > 0$. The value of the other parameter that has been used to plot this figure are $\omega_0 = 10$,Th(hot bath temperature)= 100, Tc (cold bath temperature) = 10, Gh=1,Gc=1 where the Gh and Gc are the hot and cold bath spectral function.

3.0.6 Optimization of the performance of a single spin-heat engine

Optimal protocol:

Analytically we solve for the power output P and efficiency $\eta = -P/(J_h)$ for sinusoidal modulation in section(3.4.1). Also There is an another kind of the modulation called π flip modulation, where the only two Floquet mode ($q = 0, \pm 1$) contribute to the energy heat currentHowever, there is no reason to expect that the sinusoidal or the π-flip modulation [?] results in optimal operation. So we can try to find the optimal pulse $\omega(t)$, which would maximize the power of the single spin continuous quantum heat engine. One way to do this, is to consider the CRAB method.Here we use the fact that a generic periodic modulation $\omega(t)$ can be written as a Fourier series

$$\omega(t) = w_0 + \frac{1}{2Nl(t)} \sum_{n=1}^{N} \left[a_n \cos\left(\frac{2\pi f_n t}{\tau}\right) + b_n \sin\left(\frac{2\pi f_n t}{\tau}\right) \right]. \tag{3.47}$$

Here the positive integer N represents the total number of frequencies we are considering for the CRAB optimization. Ideally N has to be infinite. However, for numerical optimization, a finite $N(N = 10, 11, \ldots 15)$ is usually enough. The function $l(t) \to \infty$ for start and end point of the cycle, while $l(t) = 1$ for intermediate times, so that $\omega(t) = \omega_0$ at the beginning and end of a cycle. This condition makes the series periodic. Notice that here the frequancy of the each term in the series are randomised to enhance the convergence of the series. We numerically optimize the Fourier coefficients $-1 \leq a_n \leq 1$, $-1 \leq b_n \leq 1$ and the randomised frequency $f_n = n(1 + r_n)$ where $-0.5 \leq r_n \leq 0.5$ so as to optimize the relevant cost function (power / efficiency / efficiency at maximum power), subject to certain constraints. The constrints could be the parameter space itself as well as outside of the parameter space such as weak coupling limit.

Optimization of the Power:

In our model the cost function that we want optimize is the power (P) of the TLS heat engine.We use equation[3.35] as the cost function. For a fixed evolution time and the temperature of the bath the power of single spin engine is the only function of the shape of the modulation $\omega(t)$. We want to find an optimal periodic pulse which would optimize the power of a two level system quantum heat engine.The optimization has been done in the following procedure:

1. First we write a general periodic modulation $\omega(t)$ in chopped random Fourier basis. Chopped means the only few number of the harmonics is considered and random basis means the frequency of the each harmonics is randomised as $\omega_k = \frac{2\pi n(1+r_n)t}{\tau}$ So $\omega(t)$ is given as,

$$\omega(t) = w_0 + \frac{\mu}{2Nl(t)} \sum_{n=1}^{10} \left[a_n \cos\left(\frac{2\pi n(1 + r_n)t}{\tau}\right) + b_n \sin\left(\frac{2\pi n(1 + r_n)t}{\tau}\right) \right]. \tag{3.48}$$

Here the Fourier series is truncated to 10 number of harmonics and instead of integer multiplied bare frequency($\frac{2\pi}{\tau}$, τ is the period of the modulation) , we have randomised frequency. Owing to the computational limit only 10 numbers of the harmonics have been considered.

2. Now the cost function P becomes a multivariate function of (a_n, b_n, r_n) and the optimization problem reduce to maximization of the function $P^{CRAB}(a_n, b_n, c_n)$ of 30 variable. Our goal is to find the value of the vector (a_n, b_n, r_n) that maximize the power.

3. CRAB optimization starts with a initial guess and then looks for the best correction. Sometimes it may get stuck at local minima so in order to avoid such scenario we use different initial guess.

In case of the sinusoidal modulation the number of the floquet mode that contribute to the heat current is 3 i.e $q = 0, \pm 1$ contribution of the other floquet mode are insignificant. But for a generic modulation we assume that number of the significant Floquet mode to be Nc where Nc is the number of the frequency used in the CRAB optimization.

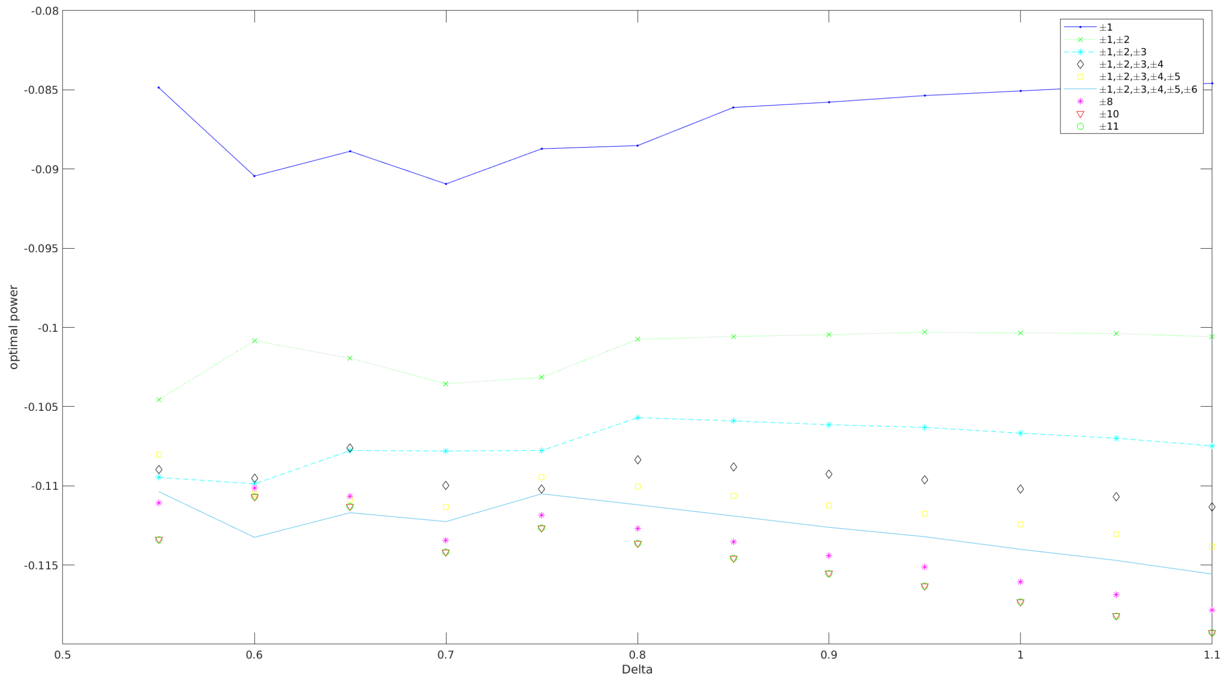

Figure 3.3: Optimal power Vs Delta for different Floquet mode

We have plotted above plot to check the number significant floquet mode that contribute to the power output for a given modulation. We observe that the optimal power output when the Floquet mode is upto ± 10 (Nc=10) converges with optimal power output of the Floquet mode upto to ± 11 . So we can conclude that in general the number of the significant Floquet mode is the value of the Nc

3.0.7 Plots and Discussion

We have considered three type of the periodic modulation to drive continuously to a TLS Hamiltonian.

1. Sinusoidal modulation
2. Random periodic modulation
3. Optimal modulation.

We observe that optimal pulse results in a better power output compared to sinusoidal and random pulse.

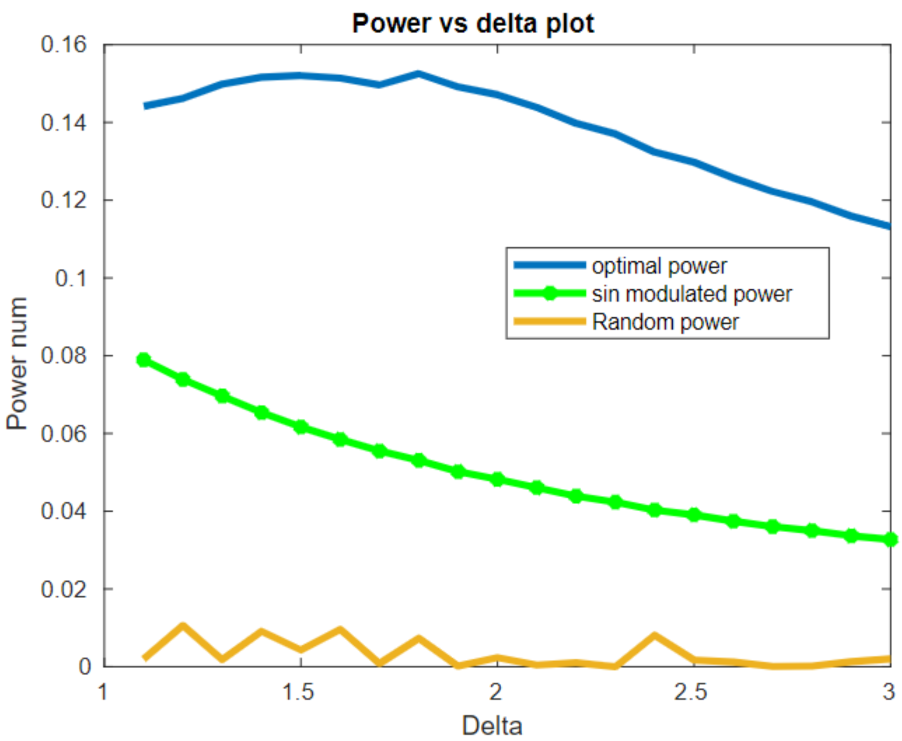

Figure 3.4: Optimal power Vs Delta for different modulation shape. We show that the optimal pulse a gives a better result comparing to the sinusoidal pulse and some random periodic pulse at every frequency of the modulation The

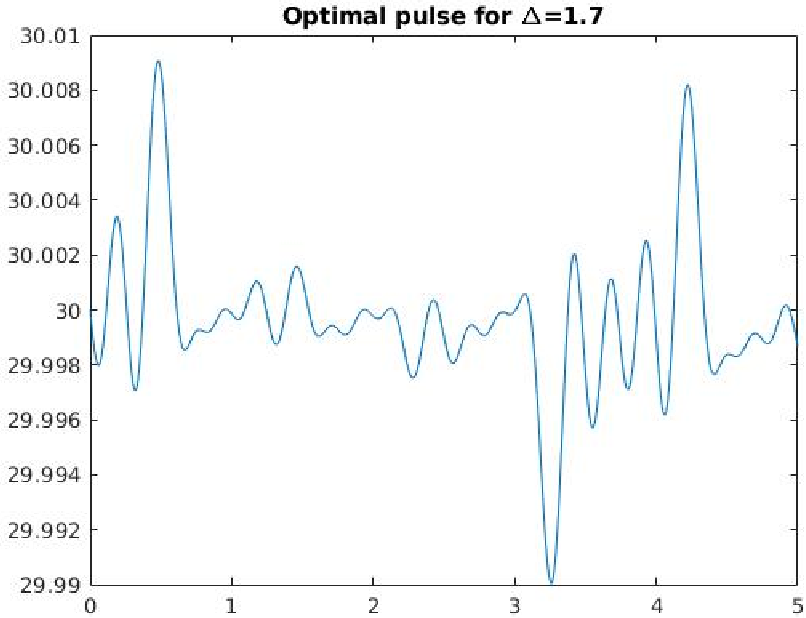

Figure 3.5: The shape of the optimal pulse at the modulating frequency $\Delta = 1.7$. The value of the ω_0 is 30 where ω_0 is the bare transition frequency of the TLS.

Chapter 4

Optimization of the continuous collective heat engine

4.0.1 Model and Set up.

Once we know the result for a single spin, we can do the same for a many-body continuous engine modelled by indistinguishable non-interacting spins, following the reference[6]. In this case we have

$$H_0 = \omega(t) J_z \tag{4.1}$$

and interaction Hamiltonisn is given by,

$$H_{Ij} = \lambda_j J_x \otimes B_j \tag{4.2}$$

where

$$J_\alpha = \sum_{r=1}^{M} \sigma_r^\alpha \tag{4.3}$$

J_α denotes the collective spin operator along dimension $\alpha = x, y, z$, and M denotes the total number of spins. The interesting properties of the collective operator is that they can be decomposed into block diagonal form,

$$J_\alpha = \bigoplus_{k=1}^{m} S_j^k \quad (\alpha \in \{x, y, z, \pm\}) \tag{4.4}$$

where the S_j^k are spin operators of lower dimension and m is the number of irreducible subspace. Hamiltonian has block diagonal form in the basis spanned by entangled many-body state. The above decomposition (4.4) comes from the theory of the spin addition[11]. The total Hilbert space of the spin ensemble can be decomposed into sum of the invariant subspace. Each invariant subspace has the dimension 2j+1 where j is the eigen value of the J^2 operator. For even number of spin-1/2 atom the value of the j are $j = 0, 1, 2 \ldots \frac{N}{2}$. N is the number of the spin-1/2 atom .When n is odd, possible value of j are $j = \frac{1}{2}, \frac{3}{2}, \frac{5}{2} \ldots \frac{N}{2}$. Using spin addition algebra, we can prove that for $N \geq 3$ there always exist the degeneracy in the subspace[15][24]. For example for N=3, the decomposition is $4 \oplus 2 \oplus 2 = 2 \otimes 2 \otimes 2$ because the the possible value of the j=1/2 and 3/2 but the space j=1/2 is 2 fold degenerate. The spin-N/2 subspace unique and comprise.We can see it for N=3, the j=3/2 subspace is unique. In collective engine, the basic assumption is that the atoms are indistinguishable and are collectively interacting with bath. Initially there is no correlation between individual atoms. Due to system-bath interaction, the bath creates quantum coherence in systems which enhance the energy current at steady state operation[6]. This generic quantum effect has common origin with dicke superradiance[25]where N optically active atom collectively interacting with a common environment like laser beam, produces the enhancement of the radiation.

4.0.2 Master Equation

GKLS equation for the reduced density matrix of the periodically modulated system can be derived using FLoquet theory[26][3][13][5][9][15].Interestingly, the master equation that we derived for the periodically modulated TLS is also valid for the N¿1 case by replacing the collective operator(4.3) instead of the single atom operator. The master equation is given by [6]

$$\dot{\rho} = \sum_{i \in \{c,h\}} \sum_{q \in \mathbb{Z}} \mathcal{L}_{i,q} \rho \tag{4.5}$$

with the sub-Liouvillians

$$\mathcal{L}_{i,q}\rho := \frac{1}{2}P(q)G_i\left(\omega_0 + q\Omega\right)\mathcal{D}\left[J_-\right] + \frac{1}{2}P(q)G_i\left(\omega_0 + q\Omega\right)\mathrm{e}^{-\beta_i\hbar(\omega_0+q\Omega)}\mathcal{D}\left[J_+\right] \tag{4.6}$$

where $\mathcal{D}[J] := 2A\rho J^\dagger - J^\dagger J\rho - \rho J^\dagger J$ denotes the dissipator. The peculiar fact about this master equation is that it conserves the symmetry of the initial prepared system expressed in the entangled many-body state[11]. This can be seen from the following fact that $[J_\pm, J^2] = 0$ and master equation involves the jump operator J^+, J^- So It does not couple the individual irreducible blocks in the density matrix and each block evolves individually. Hence, the steady-state solution of the master equation is a weighted direct sum of Gibbs-like states of these individual spin constituents,

$$\rho_{\mathrm{ss}} = \bigoplus_{m=1}^{n} \left\langle \Pi_m \right\rangle_{\rho_0} \rho_{\mathrm{ss}}^m \tag{4.7}$$

where

$$\rho_{\mathrm{ss}}^k = Z_m^{-1}\exp\left(-\beta_{\mathrm{eff}}\hbar\omega_0 S_z^m\right)$$

and

$$Z_m := \mathrm{Tr}_m\left[\exp\left(-\beta_{\mathrm{eff}}\,\hbar\omega_0 S_z^m\right)\right]$$

Here Π_m denotes the weightage of the m th invariant subspace and ρ_0 is the initial prepared system such that $\sum_{m=1}^n \left\langle \Pi_m \right\rangle_{\rho_0} = 1$ and the inverse effective temperature β_{eff} defined by the global detail balance condition[9]

$$\exp\left(-\beta_{\mathrm{eff}}\hbar\omega_0\right) := \frac{\sum_{i\in\{c,\ \mathrm{h}\}}\sum_{q\in\mathbb{Z}} P(q)G_i\left(\omega_0 + q\Omega\right)\mathrm{e}^{-\beta_i\hbar(\omega_0+q\Omega)}}{\sum_{i\in\{c,\ \mathrm{h}\}}\sum_{q\in\mathbb{Z}} P(q)G_i\left(\omega_0 + q\Omega\right)} \tag{4.8}$$

The steady state reflects the fact that the initial population weight do not change under the dynamics. each subspin relaxes to the Gibbs like state. So we can prepare our initial system such that it results in maximum collective effect when it is driven by a periodical driving force. It has been studied that when the spin-N/2 subspace subspace is populated alone in the steady state the copperative effect is maximum[6][27][24] . In this case, all N atoms behave as a single atom of spin-N/2 and this subspace is spanned by the symmetrised Dicke state[25][6][27].
The preparation of the initial state is a one time process because the symmetrised Dicke state are also energy eigenstate and the master equation doesn't change the weights of the individual spin

subspace. So once we prepare the initial state by the symmetrised Dicke basis it is guaranteed that the spin-N/2 subspace is populated in the steady state.

4.0.3 Collective Heat current and Power.

The non equilibrium steady state is maintained by the interplay between three heat current (1) cold current, (2) hot current, and (3) power. Following the theory of the thermodynamics of periodically-driven open quantum systems [26][3][17][13][9] The heat currents from the two baths to the systems are given by, $\{i = c, h\}$

$$\mathcal{J}_i = \sum_{q\in\mathbb{Z}} \hbar\left(\omega_0 + q\Delta\right) \mathrm{Tr}\left[\left(\mathcal{L}_{i,q}\rho_{\mathrm{ss}}\right) J_z\right]. \tag{4.9}$$

The above expression speaks that the bath share the photons with systems not only at frequency ω_0 but also exchanged at the Floquet sidebands $\omega_0 + q\Delta$ and thus carry different energies $\hbar\left(\omega_0 + q\Delta\right)$. Putting the steady state solution(4.7) into equation (4.9), the heat currents and the power gives

$$\begin{aligned} \mathcal{J}_i &= \sum_{m=1}^{n} \left\langle \Pi_m \right\rangle_{\rho_0} \mathcal{J}_i\left(\mathrm{j}_m\right) \\ \mathcal{P} &= \sum_{k=1}^{n} \left\langle \Pi_m \right\rangle_{\rho_0} \mathcal{P}\left(\mathrm{j}_m\right) \end{aligned} \tag{4.10}$$

where

$$\mathcal{J}_i\left(\mathrm{j}_m\right) = F\left(\mathrm{j}_m\right) \sum_{q\in\mathbb{Z}} \hbar\left(\omega_0 + q\Omega\right) P(q) G_i\left(\omega_0 + q\Omega\right) \left[\mathrm{e}^{-\beta_i\hbar(\omega_0+q\Omega)} - \mathrm{e}^{-\beta_{\mathrm{eff}}\hbar\omega_0}\right] \tag{4.11}$$

is the heat current by mth invariant subspace. and the corresponding power is given by,

$$\mathcal{P}\left(\mathrm{j}_m\right) = -\left[\mathcal{J}_c\left(\mathrm{j}_m\right) + \mathcal{J}_{\mathrm{h}}\left(\mathrm{j}_m\right)\right] \tag{4.12}$$

The factor $F(j_m)$ accounts for the enhancement of the power. this prefacotor come from the fact that the atoms are collectively interacting with the bath. It is defind as

$$F\left(\mathrm{j}_m\right):=\sum_{j=0}^{2\mathrm{j}_m-1} p_j^{\mathrm{ss},m}(j+1)\left(2\mathrm{j}_m-j\right), \tag{4.13}$$

Where $p_j^{\mathrm{ss},m}$ represents the population of the j th level of the spin- j_m particle at the effective inverse temperature β_{eff} which is define by the equation(4.8). The explicit form of equation (4.13) is given by putting the thermal state (4.7)to the equation(4.9)

$$F\left(\mathrm{j}_m\right)=\frac{\sum_{j=0}^{2j_m-1} \mathrm{e}^{-j\beta_{\text{eff}}/\omega_0}(j+1)\left(2\mathrm{j}_m-j\right)}{\sum_{j=0}^{2j_m} \mathrm{e}^{-j\beta_{\text{eff}}/\omega_0}} \tag{4.14}$$

The structure of the energy currents speaks the fact that the contribution of each spin to the energy current j_m is weighted by its population in the initial state. populations factor remains unchanged since the irreducible subspaces are dynamically invariant. The collective heat current can be expressed in terms of the heat current of the single spin because in equation (105), other than prefactor, all terms are independent of the bath index i so the collective can be writen in the simple form,

$$\mathcal{J}_i\left(\mathrm{j}_k\right)=\frac{F\left(\mathrm{j}_k\right)}{F\left(\frac{1}{2}\right)}\mathcal{J}_i\left(\frac{1}{2}\right). \tag{4.15}$$

Where, $\mathcal{J}_i\left(\frac{1}{2}\right)$ is the current induced by a single two-level atom, Correspondingly the power generated by the system is given by,

$$\mathcal{P}\left(\mathrm{j}_m\right)=\frac{F\left(\mathrm{j}_m\right)}{F\left(\frac{1}{2}\right)}\mathcal{P}\left(\frac{1}{2}\right) \tag{4.16}$$

4.0.4 Power enhancement of the collective engine.

As we mentioned that the initial atomic state preparation plays a important role in enhancement of the power output. So if the initial state starts with the subspace spanned by the fully symmetrised dicke state which implies at steady state the spin-N/2 is only populated i.e $\left\langle\Pi_m\right\rangle_{\rho_0}=1\left(j_m=\frac{N}{2}\right)$. then the engine achieves maximum cooperativity.
Once we prepare our initial system with the spin-N/2 subspace,we can compare the power output of the collective engine $\mathcal{P}_{\text{coll}}:=\mathcal{P}\left(\frac{N}{2}\right)$ and its counterpart that is the N individual spin-1/2 engine $\mathcal{P}_{\text{ind}}:=N\mathcal{P}\left(\frac{1}{2}\right)$ established by N individual atoms then fulfill the relation[6]

$$\frac{\mathcal{P}_{\text{coll}}}{\mathcal{P}_{\text{ind}}}=\frac{1}{N}\frac{F\left(\frac{N}{2}\right)}{F\left(\frac{1}{2}\right)}. \tag{4.17}$$

Equation (4.17)shows that the collective power $\mathcal{P}_{\text{coll}}$ is a consequence of quantum coherence between the N two-level atoms. The dephasing causes the destruction of the coherence of the system consequently,all atoms interact with the bath and driving field independently[6] . The power output of such an engine with N individual two-level working media equals the power output $\mathcal{P}_{\text{ind}}$ of N individual engines with a single two-level working medium.That happens with low temperature limit ,

$$\lim_{\beta_{\text{eff}}\,\hbar\omega_0\to\infty} \frac{\mathcal{P}_{\text{coll}}}{\mathcal{P}_{\text{ind}}} = 1 \tag{4.18}$$

Since the all atoms stays in the ground state in the low temperature regime. So There is no differance between collective engine and in individual N-atom engine. In the high-temperature regime,

$$\lim_{\beta_{\text{eff}}\,/\omega_0\to 0} \frac{\mathcal{P}_{\text{coll}}}{\mathcal{P}_{\text{ind}}} = \frac{N+2}{3}$$

in the high-temperature regime. The superradiant scaling behaviour $\mathcal{P}_{\text{coll}} \sim N\mathcal{P}_{\text{ind}} = N^2\mathcal{P}\left(\frac{1}{2}\right)$ is thus established for sufficiently high effective temperatures such that the spin- $N/2$ particle is considerably excited. This nonlinear scaling with the system size is a direct consequence of cooperativity between the atoms, similar to Dicke superradiance where full cooperativity between the emitters causes an inverted ensemble to radiate in the form of a short burst with peak intensity proportional to N^2[25].

In the high effective-temperature limit $\beta_{\text{eff}}\,\hbar\omega_0 \to 0$ more and more levels of the spin- $N/2$ become excited. Since the transition probabilities between its individual levels $|j\rangle$ (carrying j excitation; see appendix A of [6] are enhanced by the Clebsch-Gordan coefficients,[9][11]

$$S_-^M = \sum_{j=0}^{N-1} \sqrt{(j+1)(N-j)}|j\rangle\langle j+1|,$$

the coupling of the individual levels to the bath is increased compared to the single two-level case $\sigma_- = |g\rangle\langle e|$. These enhanced transition probabilities play a role once the corresponding levels are populated, which requires a sufficiently high effective temperature in the state. This behaviour is also reflected in the amplification function where the squared coefficients from equation are weighted by the respective thermal populations of the corresponding levels of the spin- $N/2$ particle at inverse temperature β_{eff} . We also the study the effect of the increasing number atoms on the cooperative effect. We see that when the number of the atoms increases keeping high temperature limit, the collective effects increases. But there is a saturation in number of atoms after which there is no collective effects.[6] the saturation relation is given by,

$$\lim_{N\to\infty} \frac{\mathcal{P}_{\text{coll}}}{\mathcal{P}_{\text{ind}}} = \coth\left(\frac{\beta_{\text{eff}}\hbar\omega_0}{2}\right).$$

the ideal superradiant scaling behaviour for all N is, strictly speaking, only achieved in the strict limit $\beta_{\text{eff}}\,\hbar\omega_0 \to 0$.Dicke superradiance is commonly related to intense short light pulses emitted by a collection of inverted two-level atoms . By contrast, here we rather have 'continuous' or 'persistent' superradiance.

4.0.5 Sinusoidal Modulation In collective heat engine :

We connsider the sinusoidal modulation of the form

$$\omega(t) = w_0 + g\Delta\sin(\Delta t), \tag{4.19}$$

Where $g\Delta$ is the amplitude of the sinusoidal modulation. using the same formalism that we used for the TLS working medium and the equation[] We can write the power and the heat current expression as ,

$$\begin{aligned}
\mathcal{J}_{\text{c}}\left(\mathrm{j}_m\right) &= F\left(\mathrm{j}_m\right)\hbar\left(\omega_0-\Delta\right)\left(\frac{g}{2\Delta}\right)^2 G_{\text{c}}\left(\omega_0-\Delta\right)\left[\mathrm{e}^{-\beta_{\text{c}}\hbar(\omega_0-\Delta)}-\mathrm{e}^{-\beta_{\text{eff}}\hbar\omega_0}\right]\\
\mathcal{J}_{\text{h}}\left(\mathrm{j}_m\right) &= F\left(\mathrm{j}_m\right)\hbar\left(\omega_0+\Delta\right)\left(\frac{g}{2\Delta}\right)^2 G_{\text{h}}\left(\omega_0+\Delta\right)\left[\mathrm{e}^{-\beta_{\text{h}}\hbar(\omega_0+\Delta)}-\mathrm{e}^{-\beta_{\text{eff}}\hbar\omega_0}\right]\\
\mathcal{P}\left(\mathrm{j}_m\right) &= -\left[\mathcal{J}_{\text{c}}\left(\mathrm{j}_m\right)+\mathcal{J}_{\text{c}}\left(\mathrm{j}_m\right)\right]
\end{aligned} \tag{4.20}$$

Note that the number of significant floquet mode for the sinusoidal modulation is 3 i.e $q = 0.\pm 1$ this is because the higher floquet mode do not contribute to the energy current as coupling strength g is very small. for q=0 mode P(q)=0. The choice of the bath spectral function is same as TLS sinusoidal modulation

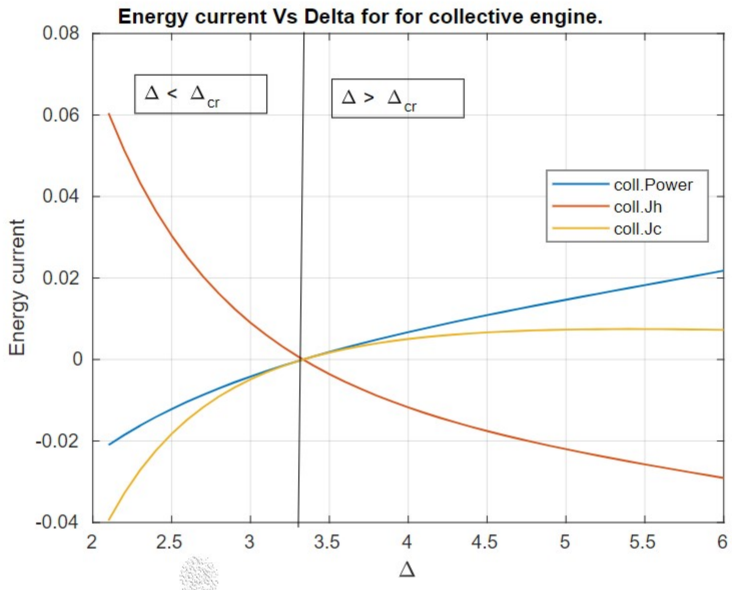

Figure 4.1: Energy current Vs Delta plot for the sinusoidal modulation. At $\Delta = \Delta_{cr}$ the operation mode changes from heat engine to refrigerator. For $\Delta > \Delta_{cr}$ the power is positive, $Jh < 0$ and $Jc > 0$. For $\Delta_{cr} < 0$, $J_h > 0$,$Jc < 0$and $P < 0$. the value of the parameters are ω_0=10, Th=100, Tc=10, Gh=1, Gc=1

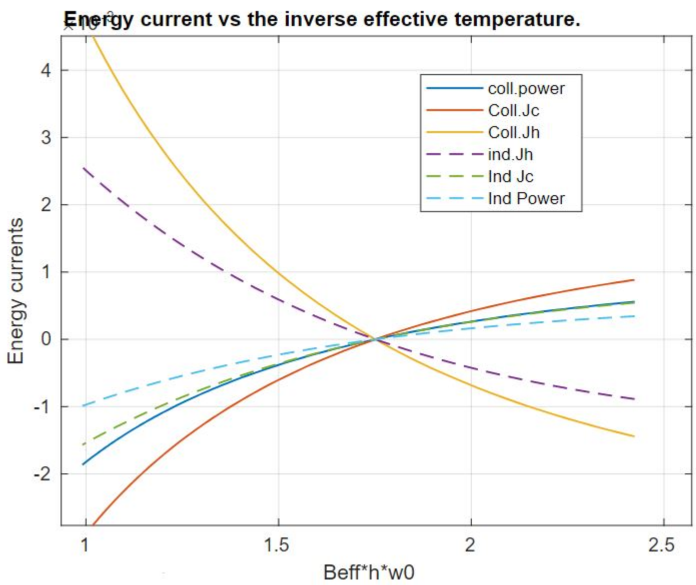

Figure 4.2: Energy current Vs inverse effective temperature plot. Plot contains the energy current of collective engine consists of 100 spin-1/2 atoms as well as the energy current of the 100 individual engine consist of the single spin-1/2 atom. We observe the collective effect here. The collective current is more compared to the individual current.

We observe the figure (4.1) follows exact same pattern as we got for the single TLS WM modulated by sinusoidal pulse (figure 3.2) . This supports our assertion that we can use the optimal pulse of the single spin heat engine to improve the power output of the collective engine. we will see more about in next session. In figure(4.2) we observe the collective effect of the engine for the sinusoidal modulation. this plot has been done for the initial system prepared by basis of the spin-N/2 subspace in order to achieve the maximum cooperative. For the low $\beta_{eff}\hbar\omega_0$ the collective effective is more prominent. Because at the high temperature regime there are more excitation and more number of atoms are collectively interact with the bath. As we decrease the temperature, collective effect is no more prominent.

4.0.6 Optimization of the Collective heat engine

It is computationally difficult to optimize the performance of many-body quantum heat engine owing to the large dimension of the corresponding Hilbert space. For N=3 system, the Hilbert space dimension becomes 2^3 So we need to handle a 8×8 matrix so as the number of the atom increases it becomes more and more difficult and the numerical optimization can be expected to take long time to run the program. . Hence , In order to overcome this problem, we propose a method to do the optimization of the many-body quantum heat engine modelled by the []
We observe the followings from the above theory :

1. The Hamiltonian of the single spin heat engine and the Hamiltonian of the multi spin heat engine are similliar. They are similiar in sense that they share the same Lie algebra.
2. Both thw Master equation has also the same structures. Both involves the jump operator and Floquet approach.

So because of this similarities we propose that we can use the optimal pulse obtained by optimizing TLS heat engine to improve the performance of the collective heat engine. Later in plot we will show that the performance of the many-body heat engine improves significantly by using the optimal pulse obtained for TLS.
We use three type of external periodic modulation to extract the power output from the collective heat engine.

1. Sinusoidal modulation
2. Random periodic Modulation

3. Previously obtained optimal pulse for single spin heat engine.(SOP-Single-atom Optimal Pulse)

We observe that ,as expected, sinusoidal modulation results in a better power output comparing to the random periodic modulation. The SOP modulation improves the engine performance significantly.This is a nice result because without even doing the optimization we got a better pulse.

Optimization of multi-spin heat engine:

In order to ensure that the SOP improves the performance, we optimize the power of the collective engine using the same protocol given in section(3). Here the cost function is the power output of the collective engine. As the CRAB requires a initial guess to start the optimization, we consider SOP as the initial guess pulse. The plot shows that the optimal pulse for the collective engine gives more power output comparing to the sinusoidal, SOP and random periodic pulse.

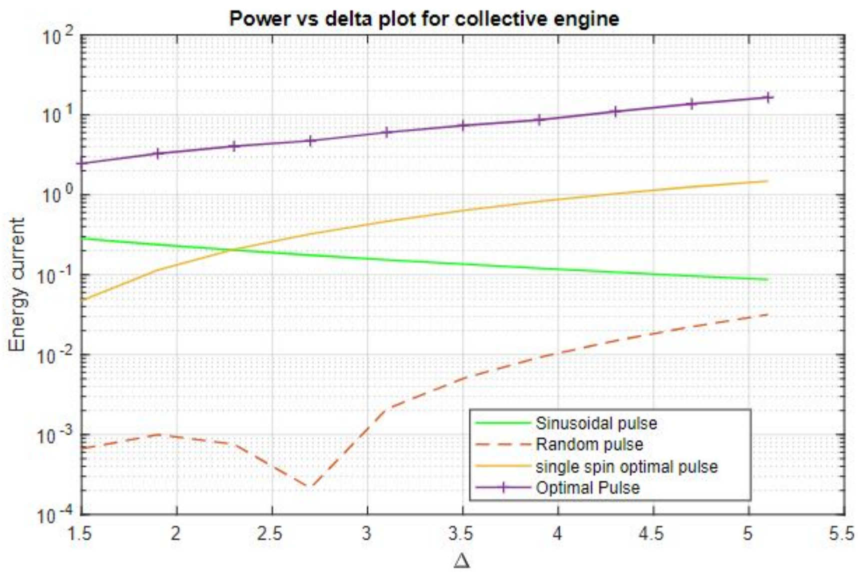

Figure 4.3: Optimal power Vs frequency of the modulation for different type of the shape of the modulation. The parameter are used as follows Th=100, Tc=10, Gh=1, Gc=1. In Y-axis the modulation of the power has been plotted in log scale. Number of the atom =100, number of the effective Floquet sideband=10,number of the frequency used in the CRAB optimization=10

4.1 Conclusion

An optimal collective continuous heat engine has many implication in the field of the quantum technology and quantum thermodynamics. But designing an optimal many body engine is yet a big challenge owing to the computational limit and the large dimension of the corresponding Hilbert space. So in my thesis work, we showed that the performance of such many-body engine can be improved significantly without doing the actual optimization. In order to achieve this we first took a small system in such a way that the dynamics and the methods are similar to the many-body system. It is computationally(Numerically) plausible to optimize the performance of the small system. So we first optimized a TLS WM heat engine and got an optimal pulse. Then we used the single spin optimal pulse for the collective engine consisting of the 100 indistinguishable non-interacting spin-1/2 atoms and we showed that the power output of the collective engines improves significantly. We also studied the quantum advantages of the collective engine due to the collective interaction with a common environment similar to the Dicke superradiance.

In order to make the perfect optimal engine one can also try to minimize the fluctuation associated with the average power and average heat current in collective engine. To do so one needs to derive a general master equation which includes the fluctuation of the work output due to the heat exchanges between bath and working medium.

Bibliography

[1] Tommaso Caneva, Tommaso Calarco, and Simone Montangero. Chopped random-basis quantum optimization. *Physical Review A*, 84(2):022326, 2011.

[2] Patrick Doria, Tommaso Calarco, and Simone Montangero. Optimal control technique for many-body quantum dynamics. *Physical review letters*, 106(19):190501, 2011.

[3] Ronnie Kosloff and Amikam Levy. Quantum heat engines and refrigerators: Continuous devices. *Annual Review of Physical Chemistry*, 65:365–393, 2014.

[4] Robert Alicki and Ronnie Kosloff. Introduction to quantum thermodynamics: History and prospects. In *Thermodynamics in the Quantum Regime*, pages 1–33. Springer, 2018.

[5] David Gelbwaser-Klimovsky, Robert Alicki, and Gershon Kurizki. Minimal universal quantum heat machine. *Physical Review E*, 87(1):012140, 2013.

[6] Wolfgang Niedenzu and Gershon Kurizki. Cooperative many-body enhancement of quantum thermal machine power. *New Journal of Physics*, 20(11):113038, 2018.

[7] Robert Alicki. Quantum thermodynamics: An example of two-level quantum machine. *Open Systems & Information Dynamics*, 21(01n02):1440002, 2014.

[8] Robert Alicki. The quantum open system as a model of the heat engine. *Journal of Physics A: Mathematical and General*, 12(5):L103, 1979.

[9] Heinz-Peter Breuer, Francesco Petruccione, et al. *The theory of open quantum systems*. Oxford University Press on Demand, 2002.

[10] Herbert B Callen. Thermodynamics and an introduction to thermostatistics. john wiley & sons. *New York*, 1985.

[11] JJ Sakurai and J Napolitano. Modern quantum physics. quantum physics, quantum information and quantum computation, 2017.

[12] Raj Kumar Pathria. *Statistical mechanics*. Elsevier, 2016.

[13] David Gelbwaser-Klimovsky, Wolfgang Niedenzu, and Gershon Kurizki. Thermodynamics of quantum systems under dynamical control. *Advances In Atomic, Molecular, and Optical Physics*, 64:329–407, 2015.

[14] Bo Xiao and Renfu Li. Finite time thermodynamic analysis of quantum otto heat engine with squeezed thermal bath. *Physics Letters A*, 382(42-43):3051–3057, 2018.

[15] Leonard Mandel and Emil Wolf. *Optical coherence and quantum optics*. Cambridge university press, 1995.

[16] D. Gelbwaser-Klimovsky, R. Alicki, and G. Kurizki. Minimal universal quantum heat machine. *Phys. Rev. E*, 87:012140, Jan 2013.

[17] SR Barone, MA Narcowich, and FJ Narcowich. Floquet theory and applications. *Physical Review A*, 15(3):1109, 1977.

[18] Christopher A Klausmeier. Floquet theory: a useful tool for understanding nonequilibrium dynamics. *Theoretical Ecology*, 1(3):153–161, 2008.

[19] Peter Abramovich Kuchment. Floquet theory for partial differential equations. *Russian Mathematical Surveys*, 37(4):1, 1982.

[20] Patrick P Hofer, Martí Perarnau-Llobet, L David M Miranda, Géraldine Haack, Ralph Silva, Jonatan Bohr Brask, and Nicolas Brunner. Markovian master equations for quantum thermal machines: local versus global approach. *New Journal of Physics*, 19(12):123037, 2017.

[21] GS Agarwal. Rotating-wave approximation and spontaneous emission. *Physical Review A*, 4(5):1778, 1971.

[22] Herbert Spohn. Entropy production for quantum dynamical semigroups. *Journal of Mathematical Physics*, 19(5):1227–1230, 1978.

[23] Vlatko Vedral. The role of relative entropy in quantum information theory. *Reviews of Modern Physics*, 74(1):197, 2002.

[24] Camille L Latune, Ilya Sinayskiy, and Francesco Petruccione. Thermodynamics from indistinguishability: Mitigating and amplifying the effects of the bath. *Physical Review Research*, 1(3):033192, 2019.

[25] Robert H Dicke. Coherence in spontaneous radiation processes. *Physical review*, 93(1):99, 1954.

[26] Ronnie Kosloff. Quantum thermodynamics: A dynamical viewpoint. *Entropy*, 15(6):2100–2128, 2013.

[27] Camille L Latune, Ilya Sinayskiy, and Francesco Petruccione. Collective heat capacity for quantum thermometry and quantum engine enhancements. *New Journal of Physics*, 22(8):083049, 2020.

[28] Wolfgang Niedenzu, Victor Mukherjee, Arnab Ghosh, Abraham G Kofman, and Gershon Kurizki. Quantum engine efficiency bound beyond the second law of thermodynamics. *Nature communications*, 9(1):1–13, 2018.

[29] Samuel J Lomonaco Jr. 102] phoenix, sjd, sm barnett, pd townsend, and kj blow, journal of modern optics (1995) 103] rarity, jg, pcm owens, and pr tapster, quantum randum-number generation and key sharing, journal of modern optics, vol. 41, no. 12, 1994, pp 2435-2444. 104] sakurai, jj,\modern quantum mechanics,"(revised edition), addison-wesley publishing com-pany, reading, massachusetts (1994). *Modern Optics*, 41(12):2455–2466, 1994.