Role of Coherence in Non-Equilibrium Quantum Thermodynamics

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Certificate of Examination

This is to certify that the dissertation titled "Role of Coherence in Non-Equilibrium Quantum Thermodynamics" submitted by Mr. Somnath Mandal(MS16065) 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.

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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 Education 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.

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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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List of Figures

Contents

Abstract

Quantum thermodynamics has opened a new world for us. It aims studying laws of thermodynamics in the quantum world. The study of open quantum systems is another benchmark that is being set in recent times. As we are inching towards making efficient quantum thermal machines, we have to encounter the problems that become dominant in quantum domain. Shortening the duration of a process leads to more power generation in the process and that introduces irreversibility in the evolution of the system. Our main interest in this thesis is to study the effects of quantum coherence in fast driving protocols, especially dividing the irreversible entropy production into two different components, coherent and non-coherent, and to study the coherent contribution in detail for different kind of driving Hamiltonians. In recent years, it has been found that the relative entropy of coherence is a useful measure of the amount of coherence generated in a system. In this thesis, we have measured relative entropy of coherence for different driving potential and studies its time dependence.

Chapter 1

Introduction

Recent advancement in nanotechnologies, miniaturization helped us building extremely small and sophisticated machines. Now as we are constantly demanding to produce smaller system it is better to know the thermodynamics of the system properly. Sometimes the system consists of only few atoms then it could not be described by the laws of thermodynamics that is used to describe system on a macroscopic point of view.

Thermodynamics could possibly be stated as one of the best theory ever produced. It is mainly developed in the 19^{th} century as the industrial revolution was taking place and humans were being replaced by machines as workforce. As people started building macroscopic engines thermodynamics became a hot topic of scientific research. At first this theory was built to understand heat to work conversion of these thermal machines but the work of Carnot has led Clasius to discover Clasius's law of thermodynamics [Thomas 11] and for the first time in the history entropy was introduced.

Meanwhile quantum theory also started developing at 20^{th} century and made huge progress throughout the last century and now believed more fundamentally accepted than classical mechanics.

The general question that would struck to any of the newcomers to this field would be - What are the requirements to simultaneously describe the quantum nature and the statistical nature of the system? Do laws of thermodynamics change in quantum domain where coherence, correlation, quantum fluctuation are dominant or remain intact? How do quantum phenomenon impacts the performance of a heat engine? How on asymptotic limit these quantum effect vanishes? How Quantum Lubrication impacts the performance of a thermal engine through an additional dephasing noise?

In thermodynamics we generally address adiabatic processes through time dependent Hamiltonians. But sometimes the internal time scale doesn't match with external time scale or the Hamiltonian doesn't commute at different times that results irreversibility in quantum system. Infinitely slow process is required to attain adiabaticity on a fundamental level. But we cannot run a thermal process for such a long time and long time process doesn't even considered as a better power resource. So for that we need to study thermal systems at finite time [Dann 20] and that's when the inner friction and irreversible work come into picture.

Generally friction could be viewed as loss of energy for moving too fast. A rapid change in any system would generate an additional entropy and will be compensated with energy cost. For example if we take a non smooth surface and try to slide a body on it , then the surface would resist and as a result of that heat will get generated and the body will eventually loose its kinetic energy and would be unable to reach its destination. Another example could be the driven gas compression process. After making it a closed system if we rapidly change the position of the piston it would cause heating in the gas and cause unwanted energy generation. To bring THE final state of the system to its quasi-static equivalent state we have to remove heat from the system. This extra work is named as frictional work.

One could ask that friction is generally a classical phenomenon so how does it work in quantum domain? How using models could we describe friction in quantum domain? As we see so many examples about quantum friction in superfluid theory , quantum cosmology etc one could ask that is friction really a quantum phenomenon or it is just classical friction embedded also in quantum domain or is there really something called quantum friction? We could see that generally quantum friction adds frictional effects beyond and above classical friction. So we a quantum system would experience more friction.

To study inner friction generated in a close quantum system we need to get the system far out from equilibrium through changing the control parameters at a finite time. As inner friction is the intrinsic properties of the system it would resist us to get to the desired result. Now the extra amount of work that we need to do in order to attain the expected result is frictional work or inner friction of the system.

The thesis is written in the following way: at first we have a chapter dedicated to understanding the basic concepts of quantum thermodynamics and quantum information theory. It would provide basic skill-set for grasping the concepts at a deeper level. In the next chapter we tried to compare finite time thermodynamic processes with infinite time reversible processes to find the correlations between these processes. Surprisingly the amount of irreversibility associated and the amount of inner friction generated could be calculated provided we know the end state of the processes. There are two cause for this generation on friction in quantum systems one is diabatic transition and another one is coherence generation between states. In the next chapter we have calculated the role of coherence in introducing irreversibility to the system. For that case we have taken a Hamiltonian and driven the system in finite time and calculated the amount of coherence generated in the process. The next chapter displays the role of coherence generating friction in quantum systems. So in our case we have taken a system and then we brought the system far from equilibrium and then measure the frictional work and relative entropy of coherence as a measure of the contribution of coherence in the frictional work.

Chapter 2

Basics of Quantum Thermodynamics

2.1 Introduction

Quantum Thermodynamics generally deals with heat, work, entropy and other thermal properties of quantum systems. This field has grown rapidly in the last two decades. Recent inclusion of equilibrium experiments and studying physical system at cold temperature and findings about the relationship between non equilibrium statistical physics and quantum information theory, resource theory has led this field to great heights. With development of fast quantum system the boundaries of limit of conventional thermodynamics is constantly getting pushed and understanding thermodynamics of these system would benefit miniaturization of technologies to nanoscale.

As this field is considered interdisciplinary in nature various perspective has emerged and each of them contributes different kinds of insight to this field. This chapter includes necessary mathematical tools that has been very useful throughout this project.

2.2 Density Operator

To describe quantum systems(open and closed) we have to incorporate the sources from where randomness is coming other than the intrinsic randomness of the system e.g, the correlations built by the system though interaction with the environment or the lack of understanding about the state of the environment that surrounds the system. Other than that we eager to know about the preparation procedure of the system to gain some insight how the system will behave under certain conditions.

Density operator describes a statistical state of a quantum system

$$\rho = \sum_{k=1}^{N} p_k \left|\psi_k\right\rangle \left\langle\psi_k\right| \tag{2.1}$$

where p_k's are the probability of the system being in the ψ_k state and $\left|\psi_k\right\rangle \left\langle\psi_k\right|$ is the projection operator on the $\left|\psi_k\right\rangle$ state. It is a positive semidefinite ($\rho \geq 0$),self adjoint($\rho = \rho^\dagger$) operator and $Tr[\rho] = 1$.
Density operator could be sufficient to calculate the outcome of the measurements correspond to an observable. Expectation value of any observable A could be written as

$$\langle A\rangle = tr(\hat{A}\hat{\rho}) = \sum_k p_k \left\langle\psi_k\right|A\left|\psi_k\right\rangle \tag{2.2}$$

2.3 Thermal State

Generally for grand canonical ensemble we have open system where energy and particle number get fluctuated then the thermal state(Gibbs state) of the system could be described by the following density matrix

$$\rho_\beta = \frac{e^{-\beta(\hat{H}-\mu\hat{N})}}{\mathrm{Tr}\left\{e^{-\beta(\hat{H}-\mu\hat{N})}\right\}} \tag{2.3}$$

Where $\hat{H}$ denotes the Hamiltonian of the system, $\hat{N}$ the particle number operator acting of the system, β the inverse temperature, μ referred as chemical potential and Z is the partition function of the system .

If a system is in equilibrium with its environment means it could exchange both particle and energy with the environment then the system could be well described by the thermal state. The thermal state maximizes Von Neumann entropy under certain conditions and it is the only completely passive state.

2.4 First and Second Laws of thermodynamics

Thermodynamics generally concerns with energy and we identify change in energy in terms of heat and work. Now, for a quantum system that is in a state ρ with Hamiltonian H the amount of internal energy or average energy of the system could be written as $\mathbf{U} = \mathrm{Tr}\{\rho H\}$. Changes in the system with respect to time brings change on the state of the system and on its Hamiltonian too. If both state and Hamiltonian($\rho^{(t)}, H^{(t)}$) changes with time on an interval $t \in [0, \tau]$, the change in systems internal energy could be

$$\Delta\mathbf{U} = \mathrm{Tr}\big(\rho^{(\tau)}H^{(\tau)}\big) - \mathrm{Tr}\big(\rho^{(0)}H^{(0)}\big) \tag{2.4}$$

The change in internal energy could generate two types of energy transfer work and heat. First one of them is fully useful and directed source of energy and the second one is not fully controllable rather could be termed as wasteful quantity. As the system Hamiltonian get changed by control parameters and could be changed in a directed way so the change in energy due to change in Hamiltonian is identified as work and the change in the state of system due to change in Hamiltonian or the correlations it builds with environment is identified as heat. By definition the heat absorbed by the system and the work done on the system could be written as

$$\langle Q\rangle = \int_0^\tau \mathrm{Tr}\Big[\dot{\rho^{(t)}}H^{(t)}\Big]dt \qquad \langle W\rangle = \int_0^\tau \mathrm{Tr}\Big[\rho^{(t)}\dot{H^{(t)}}\Big]dt \tag{2.5}$$

So the first law of thermodynamics states that mean internal energy change in a system is equal to sum of average heat and the amount of work done on the system. It's important to note that internal energy does depends only on final and initial states and corresponding Hamiltonian of the system but heat and work are path dependent quantity.

$$\langle Q\rangle + \langle W\rangle = \int_0^\tau \frac{d}{dt}\mathrm{Tr}\big(\rho^{(t)}H^{(t)}\big)dt = \mathrm{Tr}\big(\rho^{(\tau)}H^{(\tau)}\big) - \mathrm{Tr}\big(\rho^{(0)}H^{(0)}\big) = \Delta\mathbf{U} \tag{2.6}$$

The second law of thermodynamics generally governs the work extraction from a process and introduces irreversibility in thermodynamics. At 1965 Clasius first introduced a function named entropy is useful to study heat transfer from environment to system through interaction at different temperatures. If $\langle\delta Q\rangle$is the heat absorbed by the system through a reversible thermodynamic process at temperature T then entropy could be defined as

$$\Delta S_{th} = \int_{rev} \frac{\langle\delta Q\rangle}{T} \tag{2.7}$$

As any cyclic process obeys $\oint \frac{\langle\delta Q\rangle}{T} \leq 0$ with equality for reversible processes we could write the Clasius law(2^{nd} law)of thermodynamics widely known as Clasius's inequality

$$\int \frac{\langle\delta Q\rangle}{T} \leq \Delta S_{th} \quad \text{or} \quad \langle Q\rangle \leq T\Delta S_{th} \quad \text{for } T = \text{constant} \tag{2.8}$$

It just states that the net change in entropy of the system is more or equal to the heat taken by the system divided by the temperature at which the heat got exchanged.

If a system having Hamiltonian H and in contact with a thermal bath at temperature T its free energy could be written as a function of state

$$F(\rho) = U(\rho) - TS(\rho) \tag{2.9}$$

Clasius statement could be reflected as the upper bound of the extracted work

$$\langle W_{ext} \rangle = - \langle W \rangle = -\Delta U - \langle Q \rangle \leq -\Delta U + T\Delta S_{th} = -\Delta F \tag{2.10}$$

But the amount of actual work extracted would depend on the process for some process it is equal to change in free energy and for some cases it's not equal to change in free energy [Vinjanampathy 16].

2.5 Dynamics of Closed Quantum System

In quantum mechanics the state of a system is represented by state vector $|\Psi\rangle$,where $|\Psi\rangle \in \mathcal{H}$.

The time evolution of a system could easily be described by the Schrodinger Equation-

$$i\hbar\frac{d}{dt}|\Psi(t)\rangle = \hat{H(t)}|\Psi(t)\rangle \tag{2.11}$$

where $H(t)$ is the time dependent Hamiltonian of the system and the solution of the Schrodinger equation then becomes-

$$|\Psi(t)\rangle = U(t, t_0)|\Psi(t_0)\rangle \tag{2.12}$$

where $U(t, t_0)$ and $|\Psi(t_0)\rangle$ are the time evolution operator and the initial state of the system respectively. Fore-mentioned unitary operator also satisfies the relation $U(t, t_0)U^\dagger(t, t_0) = U^\dagger(t, t_0)U(t, t_0) = \mathbb{1}$.

Substituting $|\Psi(t)\rangle$ in the previous equation we get

$$i\hbar\frac{d}{dt}U(t, t_0) = \hat{H(t)}U(t, t_0) \tag{2.13}$$

From the Schrodinger we could easily derive time evoltion of the density operator and this equation is known as Liouville-Von Neumann equation

$$\frac{d\rho(t)}{dt} = -\imath\hbar[H(t), \rho(t)] \tag{2.14}$$

This equation is equivalent to the classical Liouville equation and could be written in the following form

$$\frac{d\rho(t)}{dt} = \mathcal{L}(t)\rho(t) \tag{2.15}$$

where $\mathcal{L}(t)$ is the Liouville super-operator acting on the density operator to produce a new operator

$$\mathcal{L}(t)\rho(t) = -\imath\hbar[H(t), \rho(t)] \tag{2.16}$$

If we solve the previous equation then we get a solution for the density matrix at any instantaneous time

$$\rho(t) = \mathcal{T}_{\leftarrow} e^{\int_{t_o}^{t} \mathcal{L}(s)ds} \rho(t_0) \tag{2.17}$$

For any kind of time varying Hamiltonian the Liouville super-operator also become time dependent then the solution becomes

$$\rho(t) = e^{\mathcal{L}(t-t_0)} \rho(t_0) \tag{2.18}$$

If we solve the Lieuville-Von Neumann equation we would get instantaneous density matrix as

$$\rho(t) = U(t, t_0)\rho(t_0)U^{\dagger}(t, t_0) \tag{2.19}$$

For closed and isolated system the Hamiltonian is time-independent and could be calculated through integrating this equation. If we integrate the previous equation we would get unitary in the following form-

$$U(t, t_0) = e^{-\,iH(t\,-\,t_0)/\hbar} \tag{2.20}$$

- When Hamiltonian doesn't commute at different times($[H(t_1), H(t_2)] \neq 0$)

Most of the physical process the Hamiltonian is driven by a control parameter that could be controlled externally. If the Hamiltonian contains time dependent components then it could be controlled by changing the corresponding time dependent component. In order to calculate the dynamics of a time dependent Hamiltonian $H(t)$ the evolution operator needs to be calculated. In this case the evolution operator could be expressed as

$$U(t, t_0) = \mathcal{T}_{\leftarrow} e^{-\,i/\hbar \int_{t_0}^{t} H(t')dt'} \tag{2.21}$$

If we simplify the unitary from previous equation we would get

$$U(t,t_0) = \sum_n U_n(t,t_0) = \sum_n (\frac{-i}{h})^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_{n-1}} dt_n \mathcal{T} H(t_1)H(t_2)\cdots H(t_n). \tag{2.22}$$

If we consider a system that is prepared as mixed state could be written through a density matrix ρ. At time t_0 the density matrix could be written as

$$\rho(t_0) = \sum_k p_k \left|\psi_k(t_0)\right\rangle \left\langle\psi_k(t_0)\right| \tag{2.23}$$

Where p_k's are the probabilities of the system being on $\left|\psi_k(t_0)\right\rangle$ state and $\left|\psi_k(t_0)\right\rangle$ are evolving states. Now after time t the density state(ρ_t) of the system could be defined as

$$\rho_t = \sum_k p_k U(t,t_0) \left|\psi_k(t_0)\right\rangle \left\langle\psi_k(t_0)\right| U^\dagger(t,t_0) \tag{2.24}$$

2.6 Entropy

Entropy is a key concept in information theory and it measures the amount of certainty in a system. The amount of entropy associated with an observable x could be viewed from two different perspective. First one says that the entropy of an observable would be the amount of information we gain while we measure x and the second one generally measures the uncertainty associated with it without knowing the value of x. We generally try to write entropy as a function of probability distribution.The Shanon entropy of a probability distribution could be defined as

$$S(x) = S(p_1, p_2, \ldots, p_n) = -\sum_i p_i \ln p_i \tag{2.25}$$

The Shanon entropy measures the uncertainty associated with a classical probability distribution, Von Neumann entropy measures the uncertainty associated with a density operator ρ because the entries of the matrix is the probability of the system being on the pure state. Von neumann entropy of the state ρ is defined as

$$S(\rho) = -\operatorname{Tr}(\rho \ln \rho) \tag{2.26}$$

If the density operator is spectrally decomposed on its eigenstates i.e. $\rho = \sum_i p_i \left|\psi_i\right\rangle \left\langle\psi_i\right|$ then Von Neumann entropy of the system is

$$S(\rho) = -\sum_i p_i \ln p_i \tag{2.27}$$

2.7 Relative Entropy

Relative entropy is a very useful technique that measures closeness of two probability distributions $p(x)$ and $q(x)$ over the index set x. Now the relative entropy of these two distribution is defined as

$$D(p(x)||q(x)) = \sum_x p(x) \log \frac{p(x)}{q(x)} = -S(p(x)) - \sum_x p(x) \log q(x) \tag{2.28}$$

The relative entropy of ρ and and σ is defined by

$$S(\rho||\sigma) = \mathrm{Tr}(\rho \ln \rho) - \mathrm{Tr}(\rho \ln \sigma) = -S(\rho) - \mathrm{Tr}(\rho \ln \sigma) \geq 0 \tag{2.29}$$

From Klein's inequality we could show that quantum relative entropy is always positive [Allahverdyan 05] and equals to zero when ρ equals to σ.

2.8 Distance Measures

Sometimes in quantum thermodynamics we need to know how distant two quantum states are to differentiate between the expected state and the resultant state. There are two kind of distance measures one is Trace Distance and another one is Fidelity. Fidelity generally measures the distance between two probability distributions. The fidelity between two probability distributions p_x and q_x could be written as [M. Nielsen 10]

$$F(p_x, q_x) = \sum_x \sqrt{p_x q_x} \tag{2.30}$$

To know how close two quantum states are we have to calculate the fidelity between two quantum states. So the fidelity of state ρ and σ could be defined as

$$F(\rho, \sigma) = [Tr\sqrt{\sqrt{\rho}\sigma\sqrt{\rho}}]^2 \tag{2.31}$$

2.9 Work from Coherence

To understand role of coherence in a thermodynamic process we take projection operator as a route to analyse it. Coherence is a basis dependent concept and there is no preferred basis. These projection operators(dephasing maps) maps a density state ρ that contains coherence in a particular set of eigenbasis Π_k with $k = 1, 2, 3, \ldots$ to a state $\rho \mapsto \eta := \Pi_k \rho \Pi_k$, where the coherences are removed. So the maximum extracted work from coherence could be written as

$$\langle W_{ext}^{max} \rangle = kT(S(\eta) - S(\rho)) \geq 0 \tag{2.32}$$

2.10 Conclusion

In this chapter we have learned the mathematical tools useful for studying quantum friction in details. In the next chapter we could see that irreversible work and frictional work could be represented as the relative entropy of the final state and the equilibrium states.

Chapter 3

Irreversibility and Quantum Friction in Thermodynamic Process

3.1 Introduction

Internal friction arises due to rapid change in the external parameters. An external change could result a change in the semi-classical hamiltonian of the system. If we change the control parameters slowly then Quantum Adiabatic Theorem assures that the system will be in equilibrium throughout the process. There will be no change in the energy populations and therefore the change in total energy is a result of change in energy levels. Generally such a process is called Quasistatic process and always reversible.

But if we push the system faster than its thermalization time it causes mismatch between external degrees of freedom with internal degrees of freedom then such transformations are irreversible and lead to a final state that is outside of the manifold of equilibrium states [Jarzynski 11; Esposito 09].

Though the slow processes leads to better heat to work conversion the power generation of these processes are very low compared to the fast process. As in these cases we desires better results but it also comes with its own shortcomings. The irreversibility in these processes leads to better outcome and entropy production [Esposito 10; Horowitz 13]. To study irreversibility associated with finite time adiabatic transformation and the entropy associated with it in the quantum world we would start with a system initially prepared in equilibrium. At first the state is prepared in contact to a thermal bath then isolated and the hamiltonian of the system is changed from $H(\lambda_i)$ to $H(\lambda_f)$ through a control parameter λ.

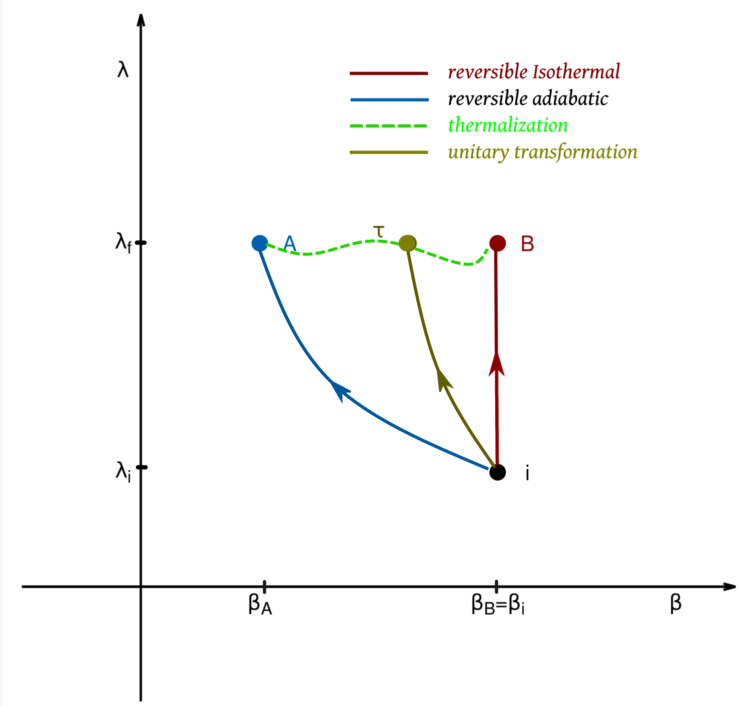

Figure 3.1: Black,Maroon,Blue points denote equilibrium states at different temperatures respectively. $\rho_i = {}^{e^{-\beta_i H_i}}/_{Z(\lambda_i,\beta_i)}$, $\rho_B = {}^{e^{-\beta_i H_f}}/_{Z(\lambda_f,\beta_i)}$, $\rho_A = {}^{e^{-\beta_A H_f}}/_{Z(\lambda_f,\beta_f)}$. The Greenish Yellow point denotes the state after the finite time $\tau, \rho_\tau = U(\tau,0)\rho_i U^\dagger(\tau,0)$

.

3.2 Irreversible Work

If the work performed on the finite time adiabatic process is w then it could be associated with a probability density function $p(w)$. In these cases the work could be lower bounded by the change in free energies between the two states and obeys Jarzynski fluctuation relation [Jarzynski 97]. As the work is lower bounded by the change in free energy(ΔF), this enforces us to introduce the concept of irreversible work that is defined through the difference in work in any finite time unitary process and the change in the free energy of the system. Generally it could be considered as a measure of the irreversibility introduced through the process.

$$\langle w_{irr}\rangle = \langle w\rangle - \Delta F \tag{3.1}$$

The process diagram is sketched in 5.1. Initially the state was in equilibrium at β_i and initial state was $\rho_i = {}^{e^{-\beta_i H_i}}/_{Z(\lambda_i,\beta_i)}$. The τ point is related with the state after the finite time unitary transformation $\rho_\tau = U(\tau,0)\rho_i U^\dagger(\tau,0)$. Other two points belongs to equilibrium states and it is shown that though the Hamiltonian of the system after three different transitions is same the τ point doesn't belongs to the same manifold of the equilibrium states.

The system starts in ρ_i with eigenbasis $\left|\epsilon_m^{(i)}\right\rangle$ and Hamiltonian H_i goes through unitary transformation and goes to H_f with eigenbasis $\left|\epsilon_m^{(f)}\right\rangle$. So the initial probability is $p_m^i = {e^{-\beta_i E_i}}/{Z(\beta_i)}$ and the transition probability is written as $p_m^{i\to f} = |\left\langle\epsilon_m^{(f)}\middle|U(\tau,0)\middle|\epsilon_m^{(i)}\right\rangle|^2$. Probability function associated with work could be written in the following way

$$p(w) = \sum_{i,f} \frac{e^{-\beta_i E_i}}{Z(\beta_i)} |\left\langle\epsilon_m^{(f)}\middle|U(\tau,0)\middle|\epsilon_m^{(i)}\right\rangle|^2 \delta(w-(E_f-E_i)) \tag{3.2}$$

The expectation value of the work done by system could be calculated using the probability distribution

$$\langle w\rangle = \sum_{m,n}(E_f-E_i)p_m^i p_m^{i\to f} = \frac{1}{\beta_B}(Tr(\rho_\tau \ln\rho_\tau) - Tr(\rho_\tau \ln\rho_B)) - \frac{1}{\beta_B}\ln\frac{Z_B}{Z_i} \tag{3.3}$$

The last term on the right hand side of the equation is equal to the change in free energy as $F = -\frac{1}{\beta}\ln Z$ and the first two terms could be defined as Kullback-Leibler divergence or relative entropy between the density operator after the time $\tau(\rho_\tau)$ and the density operator of the system after reversible isothermal process(ρ_B).

$$\langle w\rangle = \frac{1}{\beta_B}D(\rho_\tau \parallel \rho_B) + \Delta F \tag{3.4}$$

Irreversible work generated through this process is

$$\langle W_{irr}\rangle = -\Delta F + \langle w\rangle = \frac{1}{\beta_B}D(\rho_\tau \parallel \rho_B) \tag{3.5}$$

Now the amount of irreversible entropy generated throughout the process could be written as [Deffner 10]

$$\langle \Delta S_{irr}\rangle = \beta_B\langle W_{irr}\rangle = D(\rho_\tau \parallel \rho_B) \tag{3.6}$$

Using the definition of free energy we could see that the irreversible work is related to the heat required for thermalization of the system from state ρ_τ at temperature $T = \beta_B^{-1}$ as shown in [Apollaro 15]

$$\langle W_{irr}\rangle = T_B(S_B - S_i) - \left\langle Q_{\tau\to B}^{th}\right\rangle \tag{3.7}$$

where $\left\langle Q_{\tau\to B}^{th}\right\rangle = Tr\{(\rho_B - \rho_\tau)H_f\}$ is the heat taken by the system in time of thermalization. We could use these results to compare irreversible work with frictional work.

3.3 Inner Friction

On the other side of the picture we would compare our finite time adiabatic transformation $(i \to \tau)$ with reversible adiabatic transformation $(i \to A)$. While comparing finite time, performed after isolating the system would generally introduce the concept of quantum friction that is defined to be the difference in the work performed between the actual finite time adiabatic process and the ideal $(\tau \to \infty)$ reversible adiabatic process.

$$\langle w_{fric} \rangle = \langle w_\tau \rangle - \langle w_{i \to A} \rangle \tag{3.8}$$

Using the same method that is used for calculating the irreversible work and the amount of irreversible entropy generated in the process we could quantify the amount of inner friction and the entropy associated with it.

Though a ideal reversible process or for a quastatic process the Hamiltonian of the system get changed through the control parameters but the population inversion doesn't takes place. If the system started as equilibrium state then population of a eigenstate $|\epsilon^i_m\rangle$ of the Hamiltonian H_i could be written as $p^i_m = e^{-\beta_i \epsilon^i_m}/Z(\lambda_i, \beta_i)$. After the transformation the population of the states would become $p^f_m = e^{-\beta_A \epsilon^f_m}/Z(\lambda_f, \beta_A)$ for Hamiltonian H_f on its eigenbasis $\left|\epsilon^f_m\right\rangle$. Reversible adiabatic transformation processes demand no population inversion so for transformations from H_{λ_i} to H_{λ_f}

$$P^{(i)}_m = P^{(A)}_m \Rightarrow e^{-\beta_i \epsilon^{(i)}_m}/Z(\lambda_i, \beta_i) = e^{-\beta_A \epsilon^{(f)}_m}/Z(\lambda_f, \beta_A) \tag{3.9}$$

For a reversible adiabatic process work performed throughout the process could be written as mean energy difference of the final and initial state $\langle w_{i \to A} \rangle = \boldsymbol{U}_A - \boldsymbol{U}_i = \sum_m P^i_m(\epsilon^{(f)}_m - \epsilon^{(i)}_m)$.

Now from the definition of frictional work we could get a measure of frictional work through the difference of the work in the finite time of the unitary process and the ideal adiabatic process

$$\langle w_{fric} \rangle = \langle w_\tau \rangle - \langle w_{i \to A} \rangle = tr(\rho_\tau H_f) - \mathbf{U_A} = \sum_m \epsilon^{(f)}_m [\left\langle \epsilon^{(f)}_m \middle| \rho_\tau \middle| \epsilon^{(f)}_m \right\rangle - P^{(A)}_m] \tag{3.10}$$

Now the relative entropy between the state after unitary transformation ρ_τ and the state after reversible adiabatic process ρ_A is

$$D(\rho_\tau \parallel \rho_A) = Tr(\rho_\tau \ln \rho_\tau) - Tr(\rho_\tau \ln \rho_A) = \sum_m \beta_A \epsilon^{(f)}_m [\left\langle \epsilon^{(f)}_m \middle| \rho_\tau \middle| \epsilon^{(f)}_m \right\rangle - P^{(A)}_m] \tag{3.11}$$

We have calculated the irreversible work as relative entropy between two states in Eq. (3.5), it is shown that the frictional work could be quantified similarly as the relative entropy between the actual state ρ_τ and the equilibrium state after the reversible adiabatic transformation[Plastina 14].

$$\langle w_{fric} \rangle = \frac{1}{\beta_A} D(\rho_\tau \parallel \rho_A) \tag{3.12}$$

For thermalization process $\tau \to A$ the average heat taken by the system at T_a is $\beta_A \left\langle Q^{th}_{\tau \to A} \right\rangle = -\beta_A \langle w_{fric} \rangle = -D(\rho_\tau \parallel \rho_A)$

If we compare the heat exchanges between system and bath for both the cases we could get $\left\langle Q^{th}_{\tau \to A} \right\rangle - \left\langle Q^{th}_{\tau \to B} \right\rangle = U_A - U_B$ and eventually we could derive the relation between the irreversible work and frictional work.

$$\langle w_{fric} \rangle - \langle w_{irr} \rangle = (U_A - U_B) - T_i(S_A - S_B) \tag{3.13}$$

From Kelin's inequality we could say that frictional work and irreversible work are always greater than zero. We could have geometric lower bound of frictional work expressed in terms of Bures length [Deffner 10]

$$\beta_a \langle w_{fric} \rangle \geq \frac{8\mathcal{L}^2(\rho_\tau, \rho_A)}{\pi^2} \tag{3.14}$$

where for any two density matrix ρ_1 and ρ_2 $\mathcal{L}$ is expressed in terms of fidelity of these two states $\mathcal{L}(\rho_1, \rho_2) = \arccos\{\sqrt{F(\rho_1, \rho_2)}\}$. Fidelity of these two states is expressed as $F(\rho_1, \rho_2) = [Tr\{\sqrt{\sqrt{\rho_1}\rho_2\sqrt{\rho_1}}\}]^2$.

3.4 Fluctuation Theorem

Fluctuation theorem generally express universal properties of the probability distribution $p(\Phi)$ of functionals $\Phi[x(\tau)]$ like entropy, heat, work get evaluated through a fluctuating trajectory that starts with a predetermined probability distribution like $p_0(x_0)$. Often times these fluctuation theorems give most beautiful results like Jarzynski relation states that work done in any arbitrary paths would always be greater than work done in quasi-stationary process or the free energy difference between initial state and final state.

Integral Fluctuation Theorem

A non-dimensionalized functional $\Phi[x(\tau)]$ with probability distribution $p(\Phi)$ obeys the integral fluctuation theorem if

$$\left\langle e^{-\Phi} \right\rangle = \int p(\Phi) e^{-\Phi} d\Phi = 1 \tag{3.15}$$

If we use Jensen's inequality then we could find that $\Phi \geq 0$.

For quasi-stationary and reversible adiabatic process there would be no net entropy change as Von Neumann entropy of these states are the same. For fast processes unwanted diabatic transitions could occur that would eventually contribute to $\langle w_{fric} \rangle$. We could fully observe entropy production due to diabatic transitions by creating a stochastic entropic variable s that could be obtained through measuring the system through measuring the energy of the system before and after the process. If the two outcomes are $\epsilon_n^{(i)}$ and $\epsilon_m^{(f)}$ respectively then we could build the variable as

$$s = \beta_A \epsilon_m^{(f)} - \beta_i \epsilon_n^{(i)} \tag{3.16}$$

The probability density function associated with the variable s could be written as

$$P(s) = p_n^i P_{n \to m}^{\tau} \delta(s - (\beta_A \epsilon_m^{(f)} - \beta_i \epsilon_n^{(i)})) \tag{3.17}$$

Where the initial probability of the system being in $\left| \epsilon_m^{(i)} \right\rangle$ state is $p_n^i = Z_i^{-1} e^{-\beta_i \epsilon_n^{(i)}}$ and the transition probability is $P_{n \to m}^{\tau} = | \left\langle \epsilon_m^{(f)} \middle| U(\tau, 0) \middle| \epsilon_n^{(i)} \right\rangle |^2$. A fluctuation theorem associated with the variable s could be obtained [Tasaki 00]

$$\langle \exp\{-s\} \rangle = \frac{Z_A}{Z_i} \equiv \exp\{-(\beta_A F_A - \beta_i F_i)\} \tag{3.18}$$

Using Jensen's inequality($\langle \exp(f) \rangle \geq \exp(\langle f \rangle)$), we could derive that

$$\langle s \rangle \geq (\beta_A F_A - \beta_i F_i) \tag{3.19}$$

Now we would introduce a variable Σ that measures the amount of entropy produced in the actual process.The average amount of entropy produced in the system is always larger then zero and equals in quasistatic process.

$$\left\langle \sum \right\rangle = \langle s \rangle - (\beta_A F_A - \beta_i F_i) \geq 0 \tag{3.20}$$

fore-mentioned quantity Σ could be easily shown to be related with the frictional work, so

$$\left\langle \sum \right\rangle = \beta_A \langle w_{fric} \rangle = D(\rho_\tau \parallel \rho_A) \tag{3.21}$$

The combination of the free energy could be expressed through the cumulants of the distribution of the variable s taking $\ln(\langle e^{-s} \rangle)$ as the generator of the cumulants

$$-(\beta_A F_A - \beta_i F_i) = \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} C_n \tag{3.22}$$

Finally the inner friction or frictional work could be expressed as the combination of the cumulants of order more than 2.

$$\left\langle \sum \right\rangle = \beta_A \left\langle w_{fric} \right\rangle = \frac{C_2}{2} - \frac{C_3}{3!} + \dots \tag{3.23}$$

where $C_2 = \langle s^2 \rangle - \langle s \rangle^2$ is called variance and ,$C_3 = \langle s^3 \rangle - 3 \langle s^2 \rangle \langle s \rangle + 2 \langle s \rangle^3$ is called skewness etc.

3.5 Conclusion

In this chapter we have compared the closeness of actual finite time unitary processes that is brought far from equilibrium with reversible isothermal and reversible adiabatic processes. The comparison of work done in the finite time process with the ideal ones has lead to two different concepts one is irreversible work and another one is frictional work or inner friction. It is also shown that both of them are correlated to the heat exchange in the thermalization process and they are also interrelated to each other. At the end we could say that the inner friction obeys an integral fluctuation theorem that intern gives a precise idea about the inner friction.

Chapter 4

Irreversibility and Coherence

4.1 Introduction

The study of irreversibility and entropy production have been the heart of statistical theory and now in non-equilibrium thermodynamics and it claims to be equally important as before. In non-equilibrium quantum thermodynamics fluctuation theorems has been experimentally tested and used for studying irreversibility in closed system when the system performs work and work is done on system using external control parameters [Chiara 15; Dorner 13; Talkner 07]. Understanding how irreversibility emerges in a quantum system is a highly convenient issue [Tasaki 16; Kieu 04] as day by day we are intending to explore more of the quantum world and this is evident in the current progress in making thermal machines.

Role of coherence in non-equilibrium thermodynamics is extensively studied in the recent years. In this chapter we would take advantage of a recently introduced quantity called Relative Entropy of Coherence as a measure of coherence [Streltsov 17; Baumgratz 14] and study the role of coherence in irreversibility. More specifically we would divide the irreversible entropy into two portions, one of them is incoherent transitions and the other one is coherence. We would calculate the coherence generated in a finite time unitary process and study time dependency of coherence generation for a special type of Hamiltonian that we could control through external control parameters.[Francica 19]

4.2 Irreversible Work of Coherence

To study role of coherence in generation of irreversibility we would study unitary process where the systems are driven far from equilibrium from its initial state ρ_0 through some control parameters using time dependent Hamiltonian. We are as usual dealing with closed systems the process is unitary and the unitary operator is generated by the the Hamiltonian $H[\lambda(t)]$, where $\lambda(t)$ is the control parameter that changes the from $\lambda(t) = \lambda_0$ to $\lambda(t) = \lambda_f$ gradually throughout the process $[0, \tau]$. The Hamiltonian changes from $H(\lambda_0)$ to $H(\lambda_f)$ and the instantaneous Hamiltonian could be written as $H(t) = \sum_n \epsilon_n(t) |n(t)\rangle \langle n(t)|$, where $|n(t)\rangle$ is the eigenstate of the Hamiltonian at time t and $\epsilon_n(t)$ is the energy of that state.

Now we define free energy as $F_{\beta,\lambda} = -\beta^{-1} \ln Z(\beta, \lambda)$ where $Z(\beta, \lambda) = Tr\{e^{-\beta H(\lambda)}\}$, with equilibrium state at temperature β^{-1} is $\rho^{\beta(t)}_{\lambda(t)} = e^{\beta(F_{\beta,\lambda} - H(\lambda))}$. The system starts at $\rho_0 = \rho^{\beta}_{\lambda(0)}$ and goes through unitary evolution with $\rho_\tau = U_{\tau,0}(\lambda)\rho_0 U^{\dagger}_{\tau,0}(\lambda)$. As the system is closed throughout the process there is dissipation so the work done on the system by the driving parameter could be written as the mean energy difference between the final state and the initial state.

$$\langle w \rangle = Tr\{\rho_\tau H_f\} - Tr\{\rho_0 H_i\} \tag{4.1}$$

The deviation in work in actual process $\rho_0 \rightarrow \rho_\tau$ and quasi-static isothermal process is called irreversible work. An quasi-static isothermal process would bring the system to the equilibrium state at temperature β_i^{-1} and Hamiltonian H_f as referred in Fig. 5.1. Work done in this process is the change in free energy and comparing the work done in this process with actual process would give the irrversible work and from that we can derive irreversible entropy

$$\langle S_{irr} \rangle = \beta_i \langle w_{irr} \rangle = \beta_i (w - \Delta F) = D(\rho_\tau || \rho_B) \tag{4.2}$$

This irreversible entropy could be generated due to two reasons. First one is due to the population mismatch between the two states ρ_τ and ρ_B or the unwanted incoherent transitions between these two states. And the second reason is the coherence generated due to the unitary driving of the system. As for slow processes the time is too less there would possibly be no transition so all the irreversible entropy would get generated by the coherence.

To explore the role of coherence in this process we need to calculate the relative entropy of coherence of the state ρ_τ denoted by $C(\rho_\tau)$. The relative entropy of coherence is defined as

$$C(\rho_\tau) = min_{\sigma \in \mathbf{I}_\tau} D(\rho_\tau || \sigma) \tag{4.3}$$

where $\mathbf{I}_\tau$ is the set of incoherent states on the eigenbasis of the HamiltonianH_f, $|n(\tau)\rangle$.

To quantify the population mismatch of the final state ρ_τ and the state after quasi-static isothermal process we need to dephase the state with a dephasing map on the eigenbasis of the instantaneous Hamiltonian.

$$\Delta_t[\rho] = \sum_n |n(t)\rangle \langle n(t)| \rho |n(t)\rangle \langle n(t)| \tag{4.4}$$

Now it is known that the minimum in equation 4.3 is acheived when the σ state is equal to $\Delta_\tau[\rho_\tau]$ [Streltsov 17]. Now the relative entropy of coherence becomes

$$C(\rho_\tau) = D(\rho_\tau||\Delta_\tau[\rho_\tau]) = S(\Delta_\tau[\rho_\tau]) - S(\rho_\tau) \tag{4.5}$$

As the process is closed so the dynamics of the process is unitary,that means $S(\rho_\tau) = S(\rho_0) = S(\Delta_0[\rho_0])$. Then the relative entropy of coherence is coinciding with diagonal entropy as discussed in this paper by Polkovnikov [Polkovnikov 11].

Now if we write frictional work(entropy) in the form of coherence we get

$$\begin{aligned} \langle S_{irr}\rangle =& D(\rho_\tau||\rho_B) \\ =& - S(\rho_\tau) - Tr\{\rho_\tau \ln \rho_B\} \\ =& C(\rho_\tau) - S(\Delta\rho_\tau) - Tr\{\rho_\tau \ln \rho_B\} \\ =& C(\rho_\tau) + D(\Delta_\tau[\rho_\tau]||\rho_B) \end{aligned} \tag{4.6}$$

This equality tells us that the irreversible entropy either generates coherence between the states or it initiates unwanted incoherent changes that leads to population mismatch between the equilibrium state and final state and eventually takes away the state far from equilibrium.

Now if we want to calculate the coherence generated at any intermediate time $t \in [0, \tau]$ we could easily do the same calculations and get the following result

$$\beta_i \langle w_{irr}(t)\rangle = C(\rho_t) + D(\Delta_t[\rho_t]||\rho_B^{\lambda(t)}) \tag{4.7}$$

If we do a little bit of calculation we could get the expression of free energy of the system at any intermediate time through the following expression [Santos 19]

$$F(\rho_t) = F(\rho_B) + TC(\rho_t) + TD(\Delta_t[\rho_t]||\rho_B) \tag{4.8}$$

This equation shows that coherence is a part of non-equilibrium free energy of the system. That's why it is so important to study role of coherence in non-equilibrium quantum thermodynamics.

4.3 Physical Examples

To understand the role of coherence in physical systems in non-equilibrium thermodynamics we have taken a system with the following Hamiltonian as studied in [Batalhão 15; Francica 19].

$$H = \hbar w(t)[\sigma_x \cos(\phi(t)) + \sigma_y \sin(\phi(t))] \tag{4.9}$$

where $\phi(t) = \frac{\pi t}{2\tau}$ and $w(t) = w_i(1 - {}^{t}\!/\!{}_{\tau}) + w_f {}^{t}\!/\!{}_{\tau}$, is changed through the external control parameters. Here we have taken $w_f = 2w_i$. Now the system starts with Hamiltonian $H_0 = \hbar w(0)\sigma_x$ and state $\rho_0 = {}^{e^{-\beta_i H_0}}\!/\!{}_{Z}$, where $Z = Tr[e^{-\beta_i H_0}]$. Now the system undergoes an unitary transformation in time $[0, \tau]$ with final Hamiltonian $H_f = \hbar w(\tau)\sigma_y$ and the final state of the system would be $\rho_\tau = U_{(0,\tau)}\rho_0 U^\dagger_{(0,\tau)}$. We have calculated the unitary using Dyson Series and then dephased the final state ρ_τ on the eigenbasis of the final Hamiltonian. After that we have plotted relative entropy of coherence as a function of process duration τ as shown in Fig. 4.1. The second plot gives the instantaneous time dependence of the relative entropy of coherence when we fixed $w_i\tau = 1$.

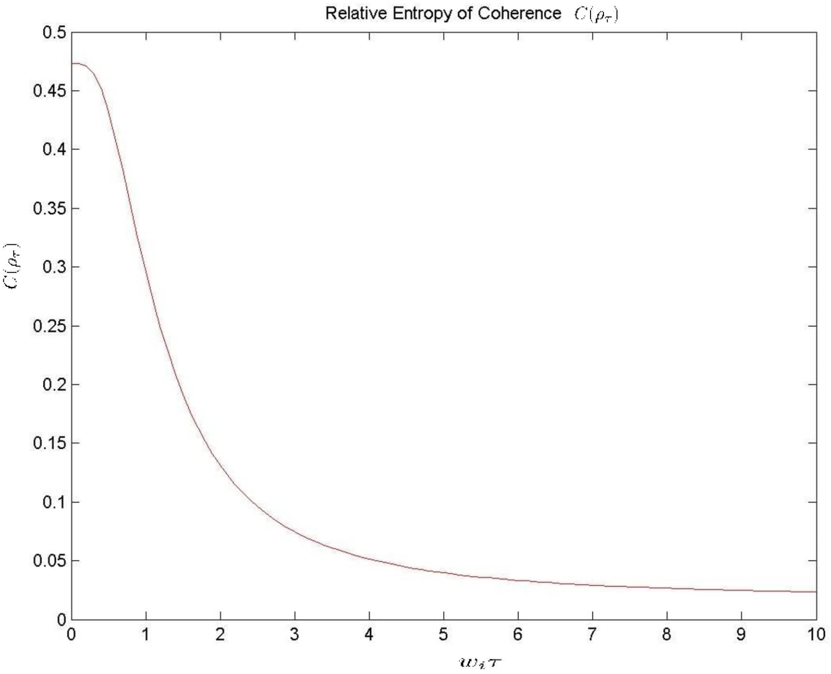

Figure 4.1: Plot of relative entropy of coherence vs total process duration, for $\beta_i\hbar w_i = 1$

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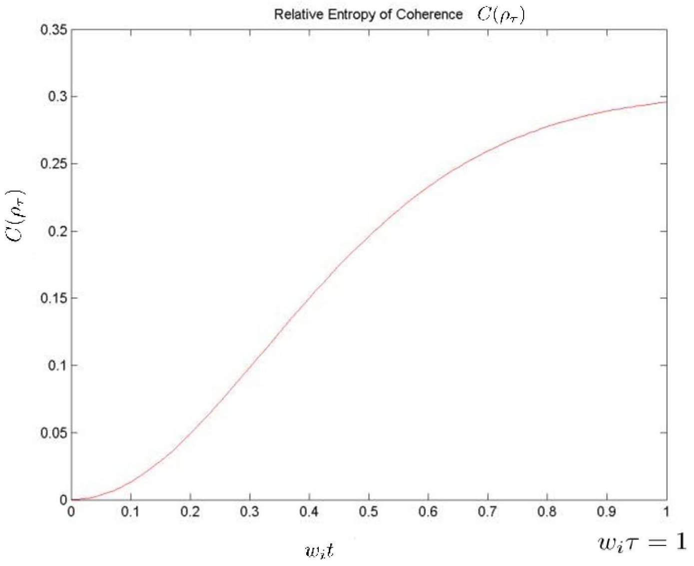

Figure 4.2: Instantaneous time dependence of relative entropy of coherence with respect to time,where $w_i\tau = 1$ and $\beta_i \hbar w_i = 2$

4.4 Conclusion

Using the concept of relative entropy of coherence we could show that coherence plays a vital role in the dynamics of non equilibrium quantum systems. Here we have studied for a model Hamiltonian but it could be studied for different time dependent Hamiltonians like, one can try to understand role of coherence in more generalized Floquet Systems. Using the same type of calculations one can study the role of coherence in generation of inner friction. It also obeys integral fluctuation theorem. One could try to make bridge between non-equilibrium quantum thermodynamics particularly quantum coherence and quantum chaos.

Chapter 5

Role of Coherence in friction

5.1 Introduction

Recent advances in nanotechnology have allowed the use of quantum heat engine for heat to work conversion and information processing purposes. Though it has its own drawbacks such as engines at those length scales don't behave classically and quantum mechanical behaviour and fluctuations becomes dominant. For finite time scale transformations, quantum friction becomes one of the undesirable features to pop up. In the present chapter, we would investigate the role of coherence in producing internal friction when the system is driven through a finite-time adiabatic transformation. It is known that coherence plays an important role in quantum phenomena and we have seen that it is the main contributor when it comes to introducing irreversibility in the system.

5.2 Physical System

We consider a system that goes through a unitary transformation using a time-dependent Hamiltonian of the form used in [Çakmak 16]

$$H(t) = B_0 I_z + B(t) I_x, \tag{5.1}$$

where B_0 is the constant magnetic field in the z direction and $B(t)$ is the time varying magnetic field applied on the x direction. I_α's are the spin angular momentum along the $\alpha(x, y, z)$ direction and they obeys the canonical commutation relation $[I_\alpha, I_\beta] = i\epsilon_{\alpha\beta\gamma} I_\gamma$. As $I_\alpha = {}^{\sigma_\alpha}\!/_2$, these operators complete a Lie algebra. In this case, we have taken $\hbar$ and Boltzmann's constant equal to unity. As from Eq. 5.1, we can calculate that the Hamiltonian doesn't commute at different times $[H(t_1), H(t_2)] = -iB_0(B(t_1) - B(t_2))I_y \neq 0$ because the applied magnetic fields are non-uniform

$B(t_1) \neq B(t_2)$. The system density matrix doesn't follow the fast changes in system Hamiltonian (controlled by an external parameter). As a result, the density matrix of the system deviates from equilibrium in a fast-driving unitary process.

This driven unitary process is divided into two parts. The first one is called forward protocol and in this case we would drive the system from an initial Hamiltonian H_i to a final Hamiltonian H_f. After that, we would reverse the process by driving the Hamiltonian from H_f to H_i. Generally, this process is known as backward protocol.

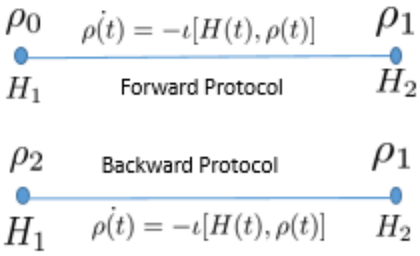

Figure 5.1: A symbolic diagram of the time evolution of the system.

- Forward Protocol

The system starts with initial Hamiltonian $H_1 = B_0 I_z + B_1 I_x$ in equilibrium at temperature $\beta^{-1} = T$. So, the initial state of the system could be written as $\rho_0 = {}^{e^{-\beta H_1}}/Z$, where $Z = Tr(e^{-\beta H_1})$. Now, the system was detached from the bath and undergoes an adiabatic transformation via a change in the time dependent magnetic field $B(t) = B_1 + (B_2 - B_1) sin(\frac{\pi t}{\tau})$. So, at time $t = 0$, the time dependent magnetic field component is $B(t = 0) = B_1$. Now, at time $t = \frac{\tau}{2}$, the time dependent magnetic field would be $B(\frac{\tau}{2}) = B_2$. At the end of the forward protocol, the Hamiltonian becomes $H_2 = B_0 I_z + B_2 I_x$ and the final density matrix becomes ρ_1. As it is an isolated process, so the evolution of the density matrix with respect to time could be defined by the unitary matrix given by the Liouville-von Neumann equation $\dot{\rho}(t) = -\iota[H(t), \rho(t)]$.

- Backward Protocol

Now in the backward protocol, the unitary process takes back the Hamiltonian from H_2 to H_1. The evolution of the density matrix with respect to time could be defined by the unitary matrix given by the Liouville-von Neumann equation $\dot{\rho}(t) = -\iota[H(t), \rho(t)]$. The time dependent component for the backward process would be $B(t) = B_2 + (B_1 - B_2)sin(\frac{\pi t}{\tau})$ with $B(t = 0) = B_2$ and $B(t = \frac{\tau}{2}) = B_1$. The final density matrix of the backward protocol is denoted by ρ_2.

5.3 Inner Friction and Coherence

From earlier chapters, we could say that the definition of frictional work is the difference between actual work and the work done in ideal diabatic process $\langle w_{fric} \rangle = \langle w_\tau \rangle - \langle w_{\tau \to \infty} \rangle$.

We have seen that it could be written as the relative entropy between the initial state and the final state $\langle w_{fric} \rangle = \beta^{-1} S(\rho_\tau \parallel \rho_{\tau \to \infty})$. The equilibrium state here would be the initial state ρ_0. If we attach a bath with the system then the heat taken by the system $\langle q_{\rho_2 \to \rho_0} \rangle$ would be equal to the frictional work.

$$S(\rho_2 \parallel \rho_0) = \beta \langle w_{fric} \rangle = -\beta \langle q_{\rho_2 \to \rho_0} \rangle \tag{5.2}$$

Frictional entropy could be written as the mean energy difference of final state and initial state times the inverse temperature $S(\rho_2 \parallel \rho_0) = \beta(tr[H_1\rho_2] - tr[H_1\rho_0])$. As we have done for irreversible work we could write the inner friction(non-adiabaticity parameter) as the sum of the coherence generation due to driving measured by $C(\rho_\tau)$ and $D(\Delta_\tau[\rho_\tau]||\rho_A)$ due to the population change in the system[Francica 19].

$$\langle S_{fric} \rangle = C(\rho_\tau) + D(\Delta_\tau[\rho_\tau]||\rho_A) \tag{5.3}$$

5.4 Results

We first calculated the Gibbs state at $\beta = 1$ with Hamiltonian $H_1 = B_0 I_z + B_1 I_x$. Then, we calculated the unitary generated by the driving pulse through Dyson Series upto second order. After that we calculated the state after forward protocol using the unitary we have calculated before. For the backward protocol, we have again calculated the unitary matrix as before. After applying the unitary to the final state after forward protocol, we got the final state of the process. We then dephased the final state on the eigenbasis of the initial Hamiltonian. Then we calculated the amount of coherence generated throughout the process using the formula stated in chapter 4. We then plotted the relative entropy of coherence as a function of total process time as shown in Fig. 5.2 for the parameters $B_0 = B_1 = 0.5$, $B_2 = 0.05$.

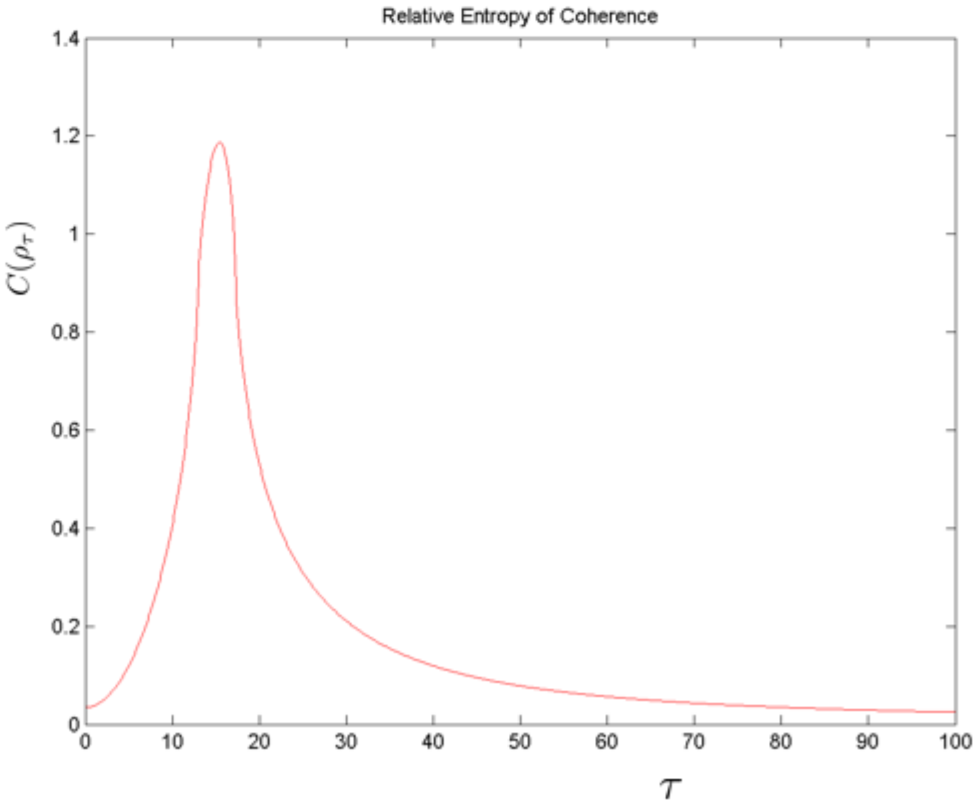

Figure 5.2: Coherence generated through the process after finite time parametric driving denoted as $C(\rho_\tau)$, as function of total process time τ.

5.5 Conclusion

The relative entropy of coherence is calculated in a simple way for a system driven out far from equilibrium. It is shown that most of the irreversibility introduced in the system is generally due to coherence building up between the states of a quantum system. We have plotted the impact on time in coherence generation in details. So we could say that transformations in finite time are irreversible in nature and a density matrix starting from an initial state never goes back to its initial state after forward-backward protocol.

Chapter 6

Conclusion and Future plans

Using the Relative Entropy of coherence, we could identify the coherent contribution to the energetics of system. Given the current interest in the field of non-equilibrium thermodynamics, relative entropy of coherence could be a vital thing to understand the details about the role of coherence in systems that are far for equilibrium. Here, we have taken different Hamiltonians driven by control parameters and studied the component of coherence generation in irreversible and frictional work and plotted them against total process time. From that data, we could see that coherence decreasing with time means that if we provide more time to the system to evolve, it would generate less coherence and eventually less irreversibility in the system.

In this project, we have talked about closed system so the dynamics of the system is unitary. We have calculated the unitary evolution operator manually using Dyson series upto second order. We think that we would get better result if we could calculate the unitary upto higher terms. Recently, we are trying to calculate the unitary through a different method where the quantum problem is addressed with analogous classical problems.

We could study the role of coherence in quantum Otto engines for different kind of Hamiltonians and calculate the impact of coherence in work done by the system or on the power generation of the system.

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