

# **THERMODYNAMIC ASPECTS OF QUANTUM COHERENCE AND CORRELATIONS**

*By*

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*A thesis submitted to the*

*Board of Studies in Physical Sciences*

*In partial fulfillment of requirements*

*for the Degree of*

**DOCTOR OF PHILOSOPHY**

*of*

**HOMI BHABHA NATIONAL INSTITUTE**



**December, 2016**



# Homi Bhabha National Institute<sup>1</sup>

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## **DECLARATION**

I, hereby declare that the investigation presented in the thesis has been carried out by me. The work is original and has not been submitted earlier as a whole or in part for a degree / diploma at this or any other Institution / University.

Avijit Misra



## List of Publications arising from the thesis

### Journal

1. “Energy cost of creating quantum coherence”, Avijit Misra, Uttam Singh, Samyadeb Bhattacharya, and Arun Kumar Pati, *Phys. Rev. A*, **2016**, 93, 052335.
2. “Quantum correlation with sandwiched relative entropies: Advantageous as order parameter in quantum phase transitions”, Avijit Misra, Anindya Biswas, Arun K. Pati, Aditi Sen(De), and Ujjwal Sen, *Phys. Rev. E*, **2015**, 91, 052125.
3. “Quantum Renyi relative entropies affirm universality of thermodynamics”, Avijit Misra, Uttam Singh, Manabendra Nath Bera, and A. K. Rajagopal, *Phys. Rev. E*, **2015**, 92, 042161.

### Further Publications of candidate not used substantially in this thesis

### Journal

4. “Generalized geometric measure of entanglement for multiparty mixed states”, Tamoghna Das, Sudipto Singha Roy, Shrobona Bagchi, Avijit Misra, Aditi Sen(De), and Ujjwal Sen, *Phys. Rev. A*, **2016**, 94, 022336.
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### Preprint

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3. “Predictive information for driven quantum systems”, *International Program on Quantum Information (IPQI-14)*, Institute of Physics (IOP), India, 17-28 February 2014.
4. “Quantum correlation with sandwiched relative entropies: Advantageous as order parameter in quantum phase transitions”, *Young Quantum-2015 (YouQu-15)*, Harish-Chandra Research Institute, India, 24-26 February 2015.
5. “Quantum thermodynamics and maximum entropy principle”, and “Generalized geometric measure of entanglement”, *Meeting on Quantum Information Processing and Applications (QIPA-15)*, Harish-Chandra Research Institute, India, 7-13 December 2015.
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Avijit Misra



**Dedicated to**

**My Parents and Family Members**



# Acknowledgments

First and foremost, I would like to take this opportunity to express my sincere gratitude towards my advisor Prof. Arun Kumar Pati for his continuous support during my Ph.D. His guidance and immense knowledge helped me in the course of my research and in writing of this thesis. I am sincerely grateful to my advisor for sharing his illuminating views on a number of problems related to this thesis.

Besides my advisor, I would like to thank Prof. Aditi Sen De, Prof. Ujjwal Sen and Prof. A. K. Rajagopal for their continuous encouragement and support. I am thankful to the members of my thesis advisory committee for their support to continue my research without any obstructions. I express my deep gratitude to the faculty members who have been instructors of the courses that I had credited at HRI. The courses were extremely helpful for me.

I would like to thank all my teachers of Asansol Old station High School, Asansol, and Ramakrishna Mission Vidyamandira, Belur Math, especially Dr. Rabindranath Sau and Dr. Dipak Ghose, who have expended their valuable time and energy and inspired me to pursue research.

I would never forget all the beautiful moments which I shared with my friends at HRI. I would like to acknowledge my batch mates and friends Swapno, Masud, Dharma, Raghu, Nyayabanta, Abhishek, Mohana, Akansha and all the friends whom I have enjoyed a lot to interact with. I would like to express my gratitude towards the whole QIC group for their support at various occasions during my Ph.D. time. It is a great pleasure to acknowledge Samyadeb, Sudipto, Debasis (Mondal, Sadhukhan), Debraj, Amit, Namrata, Uttam, Asutosh, Chiranjib, Anindita, Shrobona, Sreetama, Tamoghna, Utkarsh, Anindya, Manabendra, Prabhu with whom I had many discussions on various topics in quantum information and general physics which have proven very useful in writing this thesis.

I am immensely thankful to the administration of HRI, for their help and support. I am thankful for the HPC clusters at HRI, on which all the numerical calculations relevant to this thesis were done.

I express my heart-felt gratitude and love to Sumit da, Biltu da, Surjava da, Barnava da, Pintu da, Tojo, Santu, Sagar, Manti di and other cousins.

A special thanks to my family. I would like to express my gratitude and love from the deepest of corner of my heart to my parents, grandmother, brother and sister in law for their continuous support and encouragement.



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# Synopsis

The superposition principle in quantum physics gives rise to classically counter-intuitive traits like coherence and entanglement. Over the past several years, significant progresses have been made to establish full fledged resource theory of entanglement and quantum coherence. With the ever increasing technological advancements towards processing of small scale quantum systems and proposals of nano-scale heat engines, it is of paramount importance to investigate the thermodynamic perspectives of quantum features like coherence and quantum correlations. In the proposed thesis, we investigate the role of quantum coherence and quantum correlations in thermodynamics. The result of the proposed thesis are significantly based on the concepts of generalized entropies, namely the Rényi and the Tsallis entropies.

We highlight here the main results obtained in the proposed thesis.

- We study how much quantum coherence can be created by unitary transformations starting from a thermal state at a finite temperature with and without constraint on the amount of available free energy. These results are published in Ref. [1].
- We find that quantum correlations with sandwiched relative entropies are advantageous over other known order parameters, including entanglement and information-theoretic measures of quantum correlations to study quantum phase transitions of transverse Ising model at absolute zero temperature. These results are published in Ref. [2].
- Exploiting the generalized entropy, namely the Rényi entropy, we have established the universality of the second law of thermodynamics in generalized scenario, based on both the Carnot and the Clausius statements. These results are published in Ref. [3].

The resource theory of quantum coherence has attracted much attention and has been vibrant in recent times due to its potential applications in quantum information theoretic protocols, quantum biology and quantum thermodynamics. Since a quantum state having coherence allows transformations that are otherwise impossible and energy conservation restricts the thermodynamic processing of coherence, it can be viewed as an independent resource in thermodynamics. Considering the thermodynamic aspects of quantum coherence we explore the intimate connection between the resource theory of quantum coherence and thermodynamic limitations

on the processing of quantum coherence. In particular, we study the creation of quantum coherence by unitary transformations with limited energy. We go on even further to present a comparative investigation of creation of quantum coherence and total correlation (quantum mutual information) within the imposed thermodynamic constraints. Considering a thermally isolated quantum system initially in a thermal state, we perform an arbitrary unitary operation on the system to create coherence. First we find the upper bound on the coherence that can be created using arbitrary unitary operations starting from a fixed thermal state. Then, we show that for any finite temperature of the initial thermal state the upper bound on coherence can always be saturated and give the explicit form of the unitary transformation to achieve the same. Such a physical process will cost some amount of energy and hence it is natural to ask that if we have a limited supply of energy to invest then what is the maximal achievable coherence in such situations? We answer this question in affirmative that there always exist a unitary operation that creates maximum coherence with limited energy and give protocols for creating maximum coherence with limited energy for qubit and qutrit systems. We find that when maximal coherence is created with limited energy, the total correlation created in the process is upper bounded by the maximal coherence and vice versa. For two qubit systems we show that there does not exist any unitary transformation that creates maximal coherence and maximal total correlation simultaneously with a limited energy cost. Our results are relevant for the quantum information processing in physical systems where thermodynamic considerations cannot be ignored.

Though the study of the proposed thesis are mostly based on quantum systems at finite temperature, we also study the role of quantum correlations in quantum phase transition in transverse field Ising model at absolute zero temperature. Characterization and quantification of quantum correlation play a central role in quantum information. Entanglement, in particular, has been successfully identified as a useful resource for different quantum communication protocols and computational tasks. Moreover, it has also been employed to study cooperative quantum phenomena like quantum phase transitions in many-body systems. However, in the recent past, several quantum phenomena of multipartite systems have been discovered in which entanglement is either absent or does not play any significant role. Such phenomena motivated the search for concepts and measures of quantum correlation independent of the entanglement-separability paradigm. Introduction of quantum discord is one of the most important advancements in this direction. It is conceptualized by using the von Neumann entropy as a measure of disorder. We introduce a class of

quantum correlation measures as differences between total and classical correlations, in a shared quantum state, in terms of the sandwiched relative Rényi and Tsallis entropies. We compare our results with those obtained by using the traditional relative entropies. We find that the measures satisfy all the plausible axioms for quantum correlations. We evaluate the measures for shared pure as well as paradigmatic classes of mixed states. We show that the measures can faithfully detect the quantum critical point in the transverse quantum Ising model and find that they can be used to remove an disquieting feature of nearest-neighbor quantum discord in this respect. Furthermore, the measures provide better finite-size scaling exponents of the quantum critical point than the ones for other known order parameters, including entanglement and information-theoretic measures of quantum correlations.

Another direction of the proposed thesis is the study of quantum thermal machines which has attracted a great deal of interest in recent times. In the domain of nanothermodynamics a major question is whether a quantum heat engine, more efficient than the Carnot engine, can be realized by harnessing the quantum nature of the systems. Exploiting the generalize entropy we show that the principle of maximum entropy affirms that no engine can be more efficient than the Carnot engine even harnessing quantum resources. To establish the universality of the Carnot statement of the second law of thermodynamics, we formulate a complete theory of quantum thermodynamics in the Rényi entropic formalism exploiting the Rényi relative entropies, starting from the maximum entropy principle. In establishing the first and second laws of quantum thermodynamics, we have *correctly* identified accessible work and heat exchange both in equilibrium and non-equilibrium cases. The free energy (internal energy minus temperature times entropy) remains unaltered, when all the entities entering this relation are suitably defined. Exploiting Rényi relative entropies we have shown that this “form invariance” holds even beyond equilibrium and has profound operational significance in quantifying accessible work in isothermal process. These results reduce to the Gibbs-von Neumann results when the Rényi entropic parameter  $\alpha$  approaches 1. Moreover, it is shown that the *universality* of the Carnot statement of the second law is the consequence of the form invariance of the free energy, which is in turn the consequence of maximum entropy principle. Further, the Clausius inequality, which is the precursor to the Carnot statement, is also shown to hold based on the data processing inequalities for the traditional and sandwiched Rényi relative entropies. Thus, we find that the thermodynamics of nonequilibrium state and its deviation from equilibrium together determine the thermodynamic laws. This is another important manifestation of the concepts of in-

formation theory in thermodynamics when they are extended to the quantum realm. Our work is a substantial step towards formulating a complete theory of quantum thermodynamics and corresponding resource theory.

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# Introduction

## 1.1 Physics of information

In 1948, Claude Shannon came up with the answers of two fundamental and long standing queries of communication theory in his seminal paper “A Mathematical Theory of Communication [1].” First, how much can a message be compressed? Second, at what rate can one communicate reliably over a noisy channel? Shannon first used the tools of probability theory in communication theory. He used the concept of entropy to quantify the uncertainty in a message, which eventually grew into the field of “Information theory.” It was Shannon’s idea that one could think of information independent of the physical system that encodes it. The nature of the information in a letter, a phone call, a bit of string are the same. Due to this level of mathematical abstraction and independence over the nature of the physical system which stores the information, information theory was previously considered only as a part of communication theory which has nothing to do with physics.

Though one can conceptualize information independent of the physical system that encodes it, information processing tasks depend on the nature of the physical system that stores the information and the laws that govern evolution of the state of the physical system. Eventually, it turns out that not all information are the same in nature. Let us elaborate it further. The fundamental unit of classical information is the bit which can take one of two values: 0 and 1. For example, a sender sends either a black or white ball to the receiver to convey occurrence of one of the two possible outcomes of a dichotomous event. But the universe we live in is quantum mechanical! What if the sender encodes the information in “up” or “down” states of a spin half particle? The “up” and “down” states can be visualized as the black and

white ball: two distinguished states to encode the two outcomes. Interestingly, the spin half particle can be in a superposition of “up” and “down” states which cannot be distinguished with certainty from the “up” and “down” states. This superposition principle gives rise to classically counter intuitive traits in quantum physics. The concepts of information processing and communication significantly differs in the quantum world. One cannot copy an unknown quantum state. Therefore, it is not possible to copy the information stored in the quantum state without disturbing the system. Whereas one can make a photocopy of a letter without knowing the message written in it. Eventually, information processing tasks such as dense coding [2], teleportation [3], remote state preparation [4, 5], secure quantum communication [6, 7] have been realized which are not possible in the classical realm. With these seminal works a novel potential discipline, “Quantum information”, began to emerge in the 1980’s [8]. Given that quantum mechanics has many counter intuitive traits, one can expect that it might have a huge impact on computing. A quantum system is capable of computation was first pointed out independently by Paul Benioff and Richard Feynman in 1982. It was Peter Shor who in 1994, came up with an algorithm that offers exponential speed up in factoring a large number over the best known classical algorithm [9, 10]. Then, Lov Grover came up with a quantum algorithm in 1996, that quadratically reduces the search time [11].

Despite its enormous potential, practical applications of quantum information and computation (QIC) are still far behind than its classical counterpart. The technological advancements are still not enough to attain the full fledged quantum advantages. These technological challenges, along with the need to find out what makes the quantum protocols powerful has led to the development of resource theories of quantum entanglement. For example, in the resource theory of entanglement [12], as distributing entanglement over parties that are far apart is difficult due to loss of quantumness during the transport, all entangled states are considered as valuable resources. Thus, the states that are not entangled (separable) and the operation (local operation and classical communication) that cannot create entanglement are considered as free states and free operations. Any operation that can create entanglement between the shared quantum states is also considered as a resource. However, as the detrimental effects of the environment decohere a quantum system gradually, preserving the quantum coherence and correlations against noise for a long time is the key challenge for QIC. Therefore, to realize quantum information processing, sending information and quantum computation in its full potential, we need to have further technological advancements to manipulate and control the dynamics of the

physical systems which are small enough to possess quantum coherence and correlations. This necessity has eventually created a field of research which can be genuinely abbreviated as “Physics of information and computation.”

## 1.2 Information and thermodynamics

While quantum information and computation theory is well developed over last three decades, thermodynamics has survived crucial revolutions over the centuries. It has witnessed the advent of general theory of relativity, quantum mechanics, quantum field theories. However, it is still as relevant as it was in early days. It has often been employed to test and set benchmarks for other novel physical theories. The elegance and power of thermodynamics lie at the fact that the laws of thermodynamics do not depend on the microscopic details of the physical systems. Rather, it sets bounds on how useful a resource is, how efficiently a task can be performed, independent of the protocols and physical systems. Over the years tools of thermodynamics are being extensively employed to understand the physics of massive black holes to tiny colloids.

Despite being nascent among the physical theories, information theory has played a crucial role to solve an years old puzzle of thermodynamics, namely the work extraction by Maxwell’s demon [13, 14]. The demon uses his knowledge of the microscopic details of the system under study in extracting work that leads to apparent violation of the second law of thermodynamics. Leo Szilard studied the Maxwell’s demon problem in an idealized single atom heat engine and pointed out the significance of information in thermodynamics. Later Landauer examined the energetic cost of erasing information [15], introducing the concept of “logical irreversibility.” He formally established that “Information is physical.” Later, Bennett showed that the amount of work required in erasing demon’s memory at the end of the procedure exactly makes up for the additional work gained by the demon [16]. Thus, Landauer and Bennett put an end to the long standing debate and bridged the relationship between information and thermodynamics. The link between information theory and statistical mechanics, which underlies thermodynamics, was more formally established by E.T. Jaynes in 1957. He derived the methods of statistical mechanics using the tools of information theory [17, 18]. It was very much surprising and interesting that information theory, which was earlier thought of by the majority of researchers as an independent discipline from physical theories, played a vital role in the foundations of one of the most sacred physical theories [19, 20].

Inspired by the role of information theory in thermodynamics and noticing that both thermodynamics and quantum information theory are formulated based on how to utilize a resource most efficiently, researchers from quantum information theoretic background started exploring quantum information theory from thermodynamic perspectives. In particular, concepts of work deficit to quantify non-classical resources is an outcome of this approach. Work deficit quantifies the difference between amount of work that can be extracted globally and when the parties operate locally after suitable local transformation, from a bi-partite quantum states when it is coupled to a heat bath [21]. This work further established the intriguing link between quantum information theory and thermodynamics. Most importantly, this work has started a new direction in quantifying quantum correlations independent of entanglement-separability paradigm. The discovery of quantum discord is one of the fruitful outcomes of the same [22]. Quantum discord is given by the difference between total and classical correlation while classical correlation is given by the maximal total correlation of a post measured bipartite state. Zurek has defined quantum thermal discord taking the entropic cost of the measurement which is crucial when one considers thermodynamic perspectives [165]. Later it has been shown by Aharon and Daniel [24] that discord can determine the difference between efficiencies in Szilard's engine under different restrictions. These results have cemented the link between quantum correlations and thermodynamics. Interestingly, it has been also pointed out that the dissipated work in an irreversible process can witness entanglement [25]. With these advents, it has become a popular and fruitful practice to look into the concepts of quantum information from the thermodynamic point of view [19, 20].

### **1.3 Quantum thermodynamics: Role of quantum information**

Ever increasing technological advancements to probe and control the micro- and nanoscale systems has led to a surge of activity in the domain of nano-technology. Thermodynamics of these small scale systems become crucial from fundamental and applied perspectives. Stochastic thermodynamics [26] is one of the important domain in modern day research. It deals with the fluctuations of the thermodynamic quantities in colloids or microscopic biological systems. The famous Jarzynski [27, 28] and Crooks [29, 30] relations relate the free energy difference and the work done or extracted in transformation between states of a physical system. These relations

have been verified recently in experiments in several systems. It is of great interest to investigate what if one probes even much shorter scale where quantum effects such as coherence and entanglement are present in the system under study? To what extent the concepts of classical thermodynamics that has been instrumental in describing the macroscopic world hold in this regime? What are the striking changes that the quantum effects bring to the traditional thermodynamics? Over the last decade, these have been some important and intriguing aspects of research that have puzzled and excited the scientific community. Interestingly, it has been found that the unique entropic formulation of irreversibility of macroscopic systems is only necessary, but not sufficient to dictate the physics of small scale systems which possess quantum coherence or correlations [31, 32, 33]. It has also been observed that generalized entropies, namely the Rényi entropic formulation of the second law of thermodynamics becomes necessary in the quantum domain. The generalized relative entropies, which are key concepts in the single-shot information theory play a central role in formulating the second laws of quantum thermodynamics. To summarize, the presence of quantum coherence and correlations that are useful resources for information theoretic and technological tasks, have drastic effects on the traditional thermodynamics. Therefore, the concepts and tools of quantum information theory becoming increasingly inevitable to study quantum thermodynamics. In this newly emerged field of quantum thermodynamics, several breakthroughs have been achieved in various domains using the concepts of quantum information theory. In the following paragraphs, we briefly discuss a few research areas of quantum thermodynamics where quantum information theory has made and are still making significant contributions.

*Resource theory of quantum thermodynamics:* A resource theoretic approach to quantum thermodynamics has been of prime interest recently [31, 32, 33]. This approach aims to identify the class of operations which can or cannot be performed on quantum systems. In this resource theoretic framework, thermal operations define the set of allowed operations on a quantum system that don not change the total energy of the system and its thermal environment. Under these operations, no work can be extracted from a single heat bath. By construction, these operations are consistent with the zeroth, first and second law of thermodynamics. Interestingly, physical processes under these thermal operations impose more constraints than the ones in the classical thermodynamics. The transformation laws get more complicated in the presence of coherence in the energy eigenbasis. These resource theoretic framework provides a novel way to investigate the amount of work that can be extracted from a quantum state possessing coherence or correlation or the amount

to create quantum coherence or correlations. Thus, the resource theory of quantum thermodynamics can be far-reaching to analyze the performance of quantum thermal machine or the efficiency of thermodynamic tasks. In this resource theory of quantum thermodynamics, the concepts of quantum information theory and its mathematical tools have been instrumental and ubiquitous so far and the resource theories of quantum resources such as coherence or entanglement have significant contribution in this regard due to the structural similarities among the quantum resource theories.

*Quantum phase transition:* In 2002, it has been shown that quantum entanglement can detect quantum phase transitions in spin chains [34, 35]. These works have introduced an active domain of studying co-operative quantum phenomena in many-body quantum systems using quantum correlations. We refer the readers for comprehensive reviews and the details in Ref. [36, 37]. Understanding quantum many-body systems is one of the most challenging problems in condensed matter physics. For example, the mechanism of high- $T_C$  superconductivity is still elusive. The quantum phase transitions that are beyond Landau's paradigm are also intriguing. Tools that have been developed using the concepts of quantum information theory, such as MPS, PEPS, DMRG, MERA etc., have been playing a great role in dealing with many-particles systems providing both analytic as well as numerical insights. Thus, the interface between quantum information theory and condensed matter has become an active field study [38].

*Quantum thermal machines:* The idea of the quantum thermal machines have been around for long time [39, 40, 41]. However, the quest to find out what are truly quantum effects in quantum thermal machines is relatively recent [42]. Tools and technique of quantum information theory are being used in pursuing this quest. Whether the quantum effects can be suitably used to surpass the performance bounds set by classical thermal machines has been of great practical interest. To address this issue, one must have to identify properly the notion of heat and work in the nonequilibrium scenario. Quantum information theory provides insightful tools to define heat and work in nonequilibrium scenario based on operational and practical motivations.

*Equilibration and thermalisation:* Deriving statistical mechanics from the evolution of an isolated quantum system is an years old issue. At first sight, it may seem that thermodynamics and quantum theory are incompatible. Thermodynamics suggests us that the entropy of the universe is always increasing. Whereas quantum mechanics suggests us that the universe is evolving unitarily and hence preserves its

purity. One can bypass this apparent paradox quantum mechanically by using the idea of entanglement, “the spooky action at a distance” as abbreviated by Einstein in early days. The entropy of the physical systems grows as they get entangled with the rest of the universe. It has been also established in a rigorous way that equilibration and thermalization are intrinsic to quantum mechanics. It has been shown that equal a priori probability is a consequence of the typicality in the Hilbert spaces [19, 20]. Derving statistical mechanics, which underlies thermodynamics, from quantum theory still remains an active field of research where the tools of information theory have been instrumental.

*Fluctuation theorems:* It is interesting to note that the famous Jarzynski and Crooks relations hold unaltered in closed quantum systems [43, 44, 45] and with minor modifications in the open quantum systems [46, 47, 48]. Reducing the work fluctuations and dissipations is vital to perform a thermodynamic task efficiently. One of the main challenges in studying quantum work fluctuation relations in the laboratory is constructing the quantum work distribution, as it needs to perform projective measurement in the instantaneous energy eigenbasis of an evolving quantum system. There has been an experimental proposal [49] and a recent experimental realization [50] to measure it reliably in trapped-ion systems. Phase estimation technique which is ubiquitous in quantum optics and information, has been proposed [51, 52] to bypass the challenges faced due to the projective measurement and realized [53] in liquid state NMR setups of late, where the quantum system under study is coupled to ancillary systems and then the tomography can be done on the ancilla. This opens up a new direction to study the quantum fluctuation relations. The benefits of the positive operator valued measures (POVM), a well known concept in quantum information and quantum optics, over the projective measurements in the study of quantum fluctuation relations has also been investigated. Recently, this scheme got huge interest with promising realization in ultra cold atoms [54]. This study of quantum fluctuations can be far-reaching to measure the statistics of dissipated heat which, in turn, is very fundamental in the study of conversion of information to energy in quantum logic gates. It is also useful to estimate the required free energy in quantum computations.

*Entropy production and quantum correlations:* In nonequilibrium thermodynamics irreversible entropy production plays a central role. It is related to the loss of useful energy due to the irreversible nature of the operations. A major quest in this domain lies in whether the entropy production by a quantum operation is related to the correlations created or destroyed between the system and its thermal bath.

A general answer in this regard is still lacking. However, in the context of an open system, it has been demonstrated that the irreversible entropy production may be linked to the total correlation between the system and its thermal environment [55]. The approach followed in this work is quite similar to the formulation of Landauer’s principle proposed in Ref [56].

## 1.4 Outline of the thesis

We have already seen that quantum information plays a pivotal role in various domains of quantum thermodynamics. In particular, the thermodynamic aspects of quantum resources such as coherence and correlations is a hot cake of modern day research. In the present thesis, we mainly focus on three such directions in quantum thermodynamics where quantum coherence and correlations have significant contributions. In what follows, we provide a outline of the thesis.

- In chapter 2, we give an introduction to resource theory of quantum coherence and discuss its thermodynamic applications. Then, in chapter 3, we focus on the thermodynamic cost of creating quantum coherence. Besides how much work can be extracted from quantum states manifesting coherence and correlations, another important question is what is the thermodynamic cost of creating quantum coherence and correlations as these are useful resources for thermodynamic and quantum technological tasks. Energy cost of creating quantum correlations has been addressed recently. We consider the physical situations where the resource theories of coherence and thermodynamics play competing roles. In particular, we study the creation of quantum coherence using unitary operations with limited thermodynamic resources. We find the maximal coherence that can be created under unitary operations starting from a thermal state and find explicitly the unitary transformation that creates the maximal coherence. Since coherence is created by unitary operations starting from a thermal state, it requires some amount of energy. This motivates us to explore the trade-off between the amount of coherence that can be created and the energy cost of the unitary process. We also find the maximal achievable coherence under the constraint on the available energy. Additionally, we compare the maximal coherence and the maximal total correlation that can be created under unitary transformations with the same available energy at our disposal. We find that when maximal coherence is created with limited energy, the total correlation created in the process is upper bounded by the maximal

coherence and vice versa. For two qubit systems we show that there does not exist any unitary transformation that creates maximal coherence and maximal total correlation simultaneously with a limited energy cost.

- In chapter 4, we provide an introduction to quantum correlation measures such as the entanglement and quantum correlations beyond entanglement. Quantum discord and work deficit are two most important quantum correlation measures that are independent of entanglement-separability paradigm. These measures are conceptualized from information theoretic perspectives. Next in chapter 5, we introduce a class of quantum correlation measures as differences between total and classical correlations, in a shared quantum state, in terms of the sandwiched relative Rényi and Tsallis entropies. We find that these measures satisfy all the plausible axioms for quantum correlations. We evaluate these measures for shared pure as well as paradigmatic classes of mixed states. We show that the measures can faithfully detect the quantum critical point in the transverse quantum Ising model and find that they can be used to remove an unquieting feature of nearest-neighbor quantum discord in this respect. Furthermore, the measures provide better finite-size scaling exponents of the quantum critical point than the ones for other known order parameters, including entanglement and information-theoretic measures of quantum correlations.
- Role of quantum coherence and correlations to enhance the performance of quantum thermal machines has been a active field of research in modern times. Identifying the what is truly quantum in quantum thermal machines set a important but challenging problem. It has also been a long standing quest whether quantum thermal machines can cross the limits set by classical thermodynamics. In particular, a major question is whether a quantum heat engine, more efficient than the Carnot engine, can be realized by harnessing the quantum nature of the systems. Exploiting the generalized entropy we show in chapter 6 that the principle of maximum entropy affirms that no engine can be more efficient than the Carnot engine even harnessing quantum resources. We formulate a complete theory of quantum thermodynamics in the Rényi entropic formalism exploiting the Rényi relative entropies, starting from the maximum entropy principle. In establishing the first and second laws of quantum thermodynamics, we have *correctly* identified accessible work and heat exchange both in equilibrium and non-equilibrium cases. The free energy (internal en-

ergy minus temperature times entropy) remains unaltered, when all the entities entering this relation are suitably defined. Exploiting Rényi relative entropies we have shown that this “form invariance” holds even beyond equilibrium and has profound operational significance in isothermal process. These results reduce to the Gibbs-von Neumann results when the Rényi entropic parameter  $\alpha$  approaches 1. It is shown that the *universality* of the Carnot statement of the second law is the consequence of the form invariance of the free energy, which is in turn the consequence of maximum entropy principle. Further, the Clausius inequality, which is the precursor to the Carnot statement, is also shown to hold based on the data processing inequalities for the traditional and sandwiched Rényi relative entropies. Thus, we find that the thermodynamics of nonequilibrium state and its deviation from equilibrium together determine the thermodynamic laws. This is another important manifestation of the concepts of information theory in thermodynamics when they are extended to the quantum realm. Our work is a substantial step towards formulating a complete theory of quantum thermodynamics and corresponding resource theory.

- Finally, we conclude in chapter 7 discussing a few future directions which are interesting and important to explore.

The chapters 3, 5, 6 are based on original and published work by us. Maximum entropy principle which established the formal link between information theory and thermodynamics, has major contributions in deriving the results of chapter 3 and 6. Results of chapter 5 and 6 are established exploiting the generalized entropies. These results further strengthen the importance of the generalized entropies in quantum thermodynamics.

## 1.5 Definitions and notations

Conventions and useful quantities that have extensively used unless mentioned otherwise in this thesis are given below:

- A quantum state  $\rho$  is a Hermitian, positive semi-definite, trace one operator in the Hilbert space.
- von Neumann entropy of a quantum state  $\rho$  is  $S(\rho) = -\text{Tr}(\rho \log \rho)$ .
- Quantum relative entropy between two quantum states:  
 $S(\rho||\sigma) = -S(\rho) - \text{Tr}(\rho \log \sigma)$ .

- $\text{Tr}_A \rho_{AB} = \rho_B$ , denotes the partial trace with respect to the party  $A$ .
- The traditional quantum relative Rényi entropy between two density operators  $\rho$  and  $\sigma$ :  $S_\alpha^R(\rho||\sigma) = \frac{\log[\text{Tr}(\rho^\alpha \sigma^{1-\alpha})]}{\alpha - 1}$ .
- Sandwiched relative Rényi entropy between two density operators  $\rho$  and  $\sigma$ :  $\tilde{S}_\alpha^R(\rho||\sigma) = \frac{1}{\alpha - 1} \log \left[ \text{Tr} \left( \sigma^{\frac{1-\alpha}{2\alpha}} \rho \sigma^{\frac{1-\alpha}{2\alpha}} \right)^\alpha \right]$ .
- Boltzmann constant is set to be unity, i.e.,  $T = 1/\beta$ .



# Quantum coherence as a resource

## 2.1 Introduction

The superposition principle in quantum physics gives rise to the classically counter-intuitive traits like coherence and entanglement [12, 57]. Over the past few years, several works have been done starting from quantifying quantum superposition [58] to establishing the full fledged resource theories of coherence [57, 59, 60, 61]. The field of quantum resource theory (QRT) of coherence has been significantly advanced over past few years [62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89] and got huge interest due to its potential applications in various domains such as quantum thermodynamics, metrology, interference phenomenon, quantum biological systems and transport phenomenon, quantum algorithms, witnessing quantum correlations, detecting quantum phase transitions and several others [57]. In this chapter, we will briefly review the resource theoretic framework of quantum coherence introduced in Ref. [59] and discuss its potential applications in quantum thermodynamics.

The restrictions underlying a QRT are manifestations of the physical restrictions that govern the physical processes. For example, in the QRT of entanglement, the consideration of local operations and classical communication as the allowed operations stems from the natural limitation to implement global operations on a multipartite quantum system with parties separated apart. Any QRT is formed by identifying the relevant physical restrictions on the set of quantum operations and preparation of quantum states. In the QRT of thermodynamics the set of allowed operations is identified as the thermal operations and the only free state is the thermal state for a given fixed Hamiltonian [90, 91]. In the QRT of coherence the allowed

operations are *incoherent operations* and the free states are *incoherent states*. In this framework quantum states having non-zero coherence can be considered as useful resources. Thus, in QRT of coherence any state having a finite amount of coherence are called coherent states.

## 2.2 Incoherent states

QRT of coherence is inherently basis dependent. The reference basis with respect to which coherence is characterized and quantified depends on the physical problem under investigation. For example, the energy eigenbasis for transport phenomena and biological processes [92], or it may be the eigenbasis of the generator of an unknown phase shift in quantum metrology [93]. For an arbitrary fixed reference basis  $\{|i\rangle\}$ , the incoherent states are defined as follows

$$\sigma = \sum_i p_i |i\rangle\langle i|, \quad (2.1)$$

where  $p_i$ 's are the probability distributions with  $\sum_i p_i = 1$ . In QRT of coherence, the incoherent states are the free states. The set of incoherent states is denoted by  $\mathcal{I}$  in the present thesis.

## 2.3 Incoherent operation

Incoherent operations are those that map the set of incoherent states into itself. However, unlike incoherent states there is no unique definition of incoherent operations in the literature. Several choices are considered, motivated by practical considerations. Let us briefly review some important classes of incoherent operations.

- *Maximally incoherent operations*: Maximally incoherent operations (MIO) [58] form the largest class of incoherent operations which are defined as any complete positive trace preserving (CPTP) and non-selective map  $\mathcal{E}$  such that

$$\mathcal{E}[\mathcal{I}] \subseteq \mathcal{I}. \quad (2.2)$$

Any quantum operation can be obtained by the Stinespring dilation, which provides a way to realize the quantum operation as a global unitary operation  $U$  between the system and an ancilla in some state  $\sigma_A$ , followed by tracing out

the ancilla system, i.e.,

$$\mathcal{E}[\rho] = \text{Tr}_A[U(\rho \otimes \sigma_A)U^\dagger]. \quad (2.3)$$

However, it is important to determine whether the free set of operations in a given proposal can be understood as those that admit of a dilation in terms of the free states and free unitary couplings with, the auxiliary system. Then, such dilations can be referred as free dilations. In QRT, if an operation can be represented as in Eq. 2.3 by an incoherent ancilla state  $\sigma_A$  and an incoherent global unitary  $U$ , then the operation has a free dilation. Though MIO cannot create coherence, it is shown that these operations do not have a free dilation in general [87, 88].

- *Incoherent operations:* Incoherent operations (IO) [59] are characterized by the set of CPTP maps  $\mathcal{E}$ , having a Kraus decomposition  $\{K_n\}$  ( $\mathcal{E}[\rho] = \sum_n K_n \rho K_n^\dagger$ ,  $\sum_n K_n^\dagger K_n = \mathbf{1}$ ), such that for all  $n$  and  $\rho \in \mathcal{I}$ ,

$$\frac{K_n \rho K_n^\dagger}{\text{Tr}[K_n \rho K_n^\dagger]} \in \mathcal{I}. \quad (2.4)$$

Under IO no coherence can be generated from an incoherent state in any of the possible outcomes of such an operation. This class of operations also lack free dilation in general [87, 88].

- *Strictly incoherent operations:* The earlier two definitions of incoherent operations are based on the inability of the operation to generate coherence. Strictly incoherent operations (SIO) are defined based on the criterion that the admissible operations are not capable of utilizing the coherence present in a quantum state. To define the SIO it is necessary to define the dephasing operation  $\Delta$  such that

$$\Delta[\rho] = \sum_{i=1}^d |i\rangle\langle i| \rho |i\rangle\langle i|, \quad (2.5)$$

where  $\{|i\rangle\}$  is the reference basis and  $d$  is the dimension of the Hilbert space. An operation  $\mathcal{E}$  is a SIO if it can be decomposed in terms of incoherent Kraus operators  $\{K_n\}$ , such that the outcomes of a measurement in the reference basis of the output state are independent of the coherence of the input state

[94], i.e., in mathematical terms,

$$\langle i | K_n \rho K_n^\dagger | i \rangle = \langle i | K_n \Delta[\rho] K_n^\dagger | i \rangle. \quad (2.6)$$

The SIO as well do not have a free dilation in general [87, 88].

- *Translationally-invariant operations*: Note that the previous three operations allow permutations of the reference basis states for free. However, this might not be feasible in practical situations. For example, permuting the energy eigenbasis may cost energy. This suggests that permutations should not be considered as free operations. In translationally-invariant operations (TIO) permutations are not considered as free. In particular, given a Hamiltonian  $H$ , an operation  $\mathcal{E}$  is called TIO [95, 96, 97] if

$$e^{-iHt} \mathcal{E}[\rho] e^{iHt} = \mathcal{E}[e^{-iHt} \rho e^{iHt}]. \quad (2.7)$$

TIO plays a central role in resource theory of asymmetry and quantum thermodynamics, as we will discuss later. Importantly, TIO have a free dilation if one allows postselection with an incoherent measurement on the ancilla [88].

As MIO, IO, SIO do not have a free dilation in general, a set of incoherent operations, called physical incoherent operations (PIO), is suggested which can be implemented by an incoherent ancilla and an incoherent global unitary [87]. Additionally, these PIO allow incoherent measurement on the ancilla and classical postprocessing of the measurement outcomes. The inclusion relations between the sets of incoherent operations are complicated and in Ref. [87], it is shown that

$$\text{PIO} \subset \text{SIO} \subset \text{IO} \subset \text{MIO}. \quad (2.8)$$

Another interesting class is dephasing-covariant incoherent operations (DIO) [87, 88], which commute with the dephasing map given in Eq. 2.6. We would also like to mention genuinely incoherent operations (GIO) [85], defined as  $\mathcal{E}[|i\rangle\langle i|] = |i\rangle\langle i|$ , which are incoherent regardless of the Kraus decomposition and consider the additional constraints, such as energy preservation. In Ref. [98], a class of energy preserving operations (EPO) are defined as all operations which have free dilation as well as the global unitary commutes with the Hamiltonian of the system and ancilla individually. Note that EPO is a strict subset of TIO.

Under this framework of incoherent states and incoherent operations coherent

states are useful resources. One can create deterministically all other  $d$ -dimensional states from  $d$ -dimensional maximally coherent states by means of IO [59]. The canonical example of a maximally coherent state [59] is

$$|\phi\rangle_d = \frac{1}{\sqrt{d}} \sum_{i=1}^d |i\rangle. \quad (2.9)$$

Moreover, maximally coherent states allow generation of any quantum operations via IO [59, 87]. As coherent states are useful resources it is essential to quantify the resource content of a coherent state. In next section, we quantify quantum coherence.

## 2.4 Quantifying coherence

A bona-fide coherence measure  $C(\rho)$  for a density operator  $\rho$  should satisfy the following properties as discussed in Ref. [59].

- *Property 1* Non-negativity:

$$C(\rho) \geq 0. \quad (2.10)$$

The equality holds only if  $\rho$  is incoherent.

- *Property 2* Monotonicity: For any incoherent operation  $\mathcal{E}$  one should have

$$C(\rho) \geq C(\mathcal{E}[\rho]). \quad (2.11)$$

- *Property 3* Strong monotonicity:  $C(\rho)$  is also non-increasing on average under selective incoherent operations,

$$C(\rho) \geq \sum_i q_i C(\sigma_i), \quad (2.12)$$

where  $q_i = \text{Tr}[K_i \rho K_i^\dagger]$  are the probabilities,  $\sigma_i = \frac{K_i \rho K_i^\dagger}{q_i}$  are the post measurement states and  $\{K_i\}$  are the incoherent Kraus operators.

- *Property 4* Convexity:  $C(\rho)$  is convex over the mixing parameters of the state, i.e., for  $\rho = \sum_i p_i \rho_i$  one has

$$\sum_i p_i C(\rho_i) \geq C(\sum_i p_i \rho_i), \quad (2.13)$$

where  $\{p_i\}$  forms a probability distribution.

Property 1 and 2 are minimal requirements to quantify a resource. Note that Property 3 and 4 together imply Property 2. A quantity  $C(\rho)$  which satisfies Property 1 and either Property 2 or Property 3 or both, is a coherence monotone. Recently, following the standard notions of resource theory of entanglement it has been proposed that a quantity  $C(\rho)$  should satisfy the following two more properties along with Property 1-4, before one calls it a coherence measure [57],

- *Property 5* Uniqueness for pure states: It has been argued in [57], to be a good measure of coherence  $C(\rho)$  should satisfy the following condition

$$C(|\psi\rangle) = S(\Delta[|\psi\rangle\langle\psi|]), \quad (2.14)$$

for any pure state  $|\psi\rangle$ , i.e., for pure states the measure is unique. It is worth noticing that the R.H.S of the above equation is relative entropy of coherence which will be discussed in detail in section 2.4.1. This condition is demanded considering the fact that the distillable coherence of a pure state is given by relative entropy of coherence in the asymptotic limit. Though one can argue that this is indeed a strong condition as the relative entropy of coherence is the amount of distillable coherence only in the asymptotic limit.

- *Property 6* Additivity:  $C(\rho)$  is additive under tensor product of quantum state,

$$C(\rho \otimes \sigma) = C(\rho) + C(\sigma). \quad (2.15)$$

The two quantifiers which satisfies Property 1-6 are, namely, the distillable coherence and the coherence cost [94]. The distillable coherence is the optimal rate of extracting maximally coherent single-qubit states  $|\phi_2\rangle$  from a given quantum state via incoherent operations in the asymptotic limit. It can be shown that the distillable coherence is equal to the relative entropy of coherence [94], which was introduced in Ref. [59] and will be discussed in detail in this thesis shortly. The coherence cost which is also the coherence of formation, following the same footing of entanglement of formation, is the minimal rate of maximally coherent single-qubit states  $|\phi_2\rangle$  required to produce a given quantum state via incoherent operations in the asymptotic limit. There are several coherence monotones in the literature which satisfy Property 1-2 and some of them also satisfy Property 3-4 as well. See the excellent review for details [57]. However, very recently a refinement over Ref. [59] on the properties that a coherence measure should satisfy has been proposed in Ref. [89]. This refinement imposes an extra condition on the measures of coherence such that the set of

states having maximal coherence value with respect to the coherence measure and the set of maximally coherent states, as defined in Ref. [59], should be identical. In this thesis, we consider the relative entropy of coherence as a measure of quantum coherence which enjoys various operational interpretations [75, 94]. Moreover, it also satisfies the additional requirement as proposed in Ref. [89].

### 2.4.1 Relative entropy of coherence

A quantifier of quantum coherence based on the distance between quantum states is defined as [59]

$$C_D(\rho) = \inf_{\sigma \in \mathcal{I}} D(\rho, \sigma), \quad (2.16)$$

where  $D$  is a contractive distance measure such that  $D(\rho, \sigma) \geq D(\mathcal{E}[\rho], \mathcal{E}[\sigma])$ . If the distance  $D$  is taken to be the quantum relative entropy then the Eq. 2.16 reduces to

$$C_r(\rho) = \inf_{\sigma \in \mathcal{I}} S(\rho \parallel \sigma). \quad (2.17)$$

Now  $S(\rho \parallel \sigma) = S(\rho^D) - S(\rho) + S(\rho^D \parallel \sigma)$  [59], as  $\sigma \in \mathcal{I}$ . Here  $\Delta[\rho] = \rho^D$ . From now on we denote the dephased state  $\Delta[\rho]$  in the reference basis as  $\rho^D$  through out the thesis. As always  $S(\rho^D \parallel \sigma) \geq 0$ , and minimum value occurs when  $\sigma = \rho^D$ . Therefore, the relative entropy of coherence of  $\rho$  is given as

$$C_r(\rho) = S(\rho^D) - S(\rho). \quad (2.18)$$

We have mentioned earlier relative entropy of coherence satisfies all of the Properties 1-6. We provide an operational quantifier of the coherence of a quantum system in terms of the amount of noise that has to be injected into the system in order to fully decohere it in Ref. [75]. This quantifies the erasure cost of quantum coherence. We employ the entropy exchange between the system and the environment during the decohering operation (an ensemble of random (in)coherent unitaries  $\{p_i, U_i\}$ ) and the space required to identify uniquely the indices “ $i$ ” appearing in the decohering operation as the quantifiers of noise. Both yield the same cost of erasing coherence in the asymptotic limit. In particular, we find that in the asymptotic limit, the minimum amount of noise that is required to fully decohere a quantum system, is equal to the relative entropy of coherence. This holds even if we allow for the nonzero small errors in the decohering process. As a consequence, it establishes that the relative entropy of coherence is endowed with an operational interpretation which may be thermodynamically meaningful too.

Moreover, it has been shown that relative entropy of coherence is related to the deviation of a quantum state from its thermal equilibrium [99]. Possible quantifiers of coherence based on the generalized relative entropy distances have been recently proposed [100]. Other remarkable distance based coherence quantifiers available in the literature are coherence quantifiers based on matrix norms [59] (mainly  $l_1$ -norm of coherence). There have also been other proposals to quantify quantum coherence which enjoys various properties to be a good coherence measure. Coherence monotone from entanglement [62], robustness of coherence [101, 102], coherence of assistance [82] are worth mentioning in this regard.

## 2.5 Application of quantum coherence

### 2.5.1 Quantum thermodynamics

Recently, various important aspects of coherence have been established in quantum thermodynamics. In what follows, we discuss a few domains where quantum coherence plays a pivotal role.

#### 2.5.1.1 State conversion via thermal operations

Inter-convertibility of two quantum states under a certain class of operations, called thermal operations, has attracted immense interest and led to a surge of activity due to its foundational importance and mathematical elegance. Astonishingly, it has been revealed that the state transformation laws under these thermal operations in the quantum domain cannot be sufficiently described by a single entropic formalism which can completely describe the allowed transformations for the macroscopic systems in thermal environment. It has been found that it is only necessary but not sufficient to dictate the transformation laws of quantum particles where the quantum coherence and correlations prevail. This demands a set of restrictions in terms of generalized entropy, namely, the Rényi entropy. In the following, we review the role of quantum coherence in the context of thermal operations.

*Thermal operations:* A thermal operation  $\mathcal{E}_T$  is defined as follows

$$\mathcal{E}_T(\rho) = \text{Tr}_b[U(\rho \otimes \gamma_T^b)U^\dagger], \quad (2.19)$$

where  $\gamma_T^b = e^{-\beta H_b} / \text{Tr}[e^{-\beta H_b}]$  is the thermal state of the environment,  $[U, H \otimes \mathbb{I} + \mathbb{I} \otimes H_b] = 0$ ,  $U$  is a joint unitary on the system and bath,  $H$  and  $H_b$  are the Hamiltonian

of the system and the bath respectively. Note that we have not used any subscript to denote the system parameters. More general formalism of thermodynamic process involves time dependent Hamiltonian. However, as already pointed out in Ref. [31, 103] that this formalism can encompass such cases by inclusion of clock degrees of freedom. The unitary operation preserves the total energy of the system and bath. One of the main property of the thermal map is that it preserves the thermal state,  $\mathcal{E}_T(\rho_T) = \rho_T$ . These two aforesaid properties are consistent with the first and second law of thermodynamics respectively.

It is worth mentioning that the thermal operations  $\mathcal{E}_T$  are TIO with respect to the system Hamiltonian  $H$  as

$$e^{-iHt}\mathcal{E}_T[\rho]e^{iHt} = \mathcal{E}_T[e^{-iHt}\rho e^{iHt}]. \quad (2.20)$$

*Second laws of quantum thermodynamics:* There have been many explorations to inquire the transformation law or laws under the aforesaid thermal operations. In Ref. [91], the condition of interconversion between two incoherent quantum states has been established. This condition is termed as *thermo-majorization*. However, one may use a catalytic transformation. An auxiliary system  $\chi_{cat}$  may allow the transformation  $\rho \otimes \chi_{cat} \rightarrow \sigma \otimes \chi_{cat}$ , though the transformation  $\rho \rightarrow \sigma$  is forbidden. Transformation laws which consider more generalized scenarios such as catalytic transformations have been established in Ref.[31]. These conditions are called *second laws of quantum thermodynamics*. The second laws of quantum thermodynamics tell us that a transformation from  $\rho$  to  $\sigma$  is only possible when the generalized free energies decrease, i.e.,

$$\Delta F_\alpha \leq 0, \quad \forall \alpha \geq 0. \quad (2.21)$$

Here, the generalized free energy of a quantum state  $\rho$  is defined as follows

$$\begin{aligned} F_\alpha(\rho, H) &= TS_\alpha^R(\rho||\rho_T^H) - T \log Z_H, \quad \text{when } \alpha \in [0, 1), \\ &= T\tilde{S}_\alpha^R(\rho||\rho_T^H) - T \log Z_H, \quad \text{when } \alpha \geq 1. \end{aligned} \quad (2.22)$$

Here,  $S_\alpha^R(\rho||\rho_T^H)$  and  $\tilde{S}_\alpha^R(\rho||\rho_T^H)$  are the traditional and sandwiched relative Rényi entropies as defined in Sec.1.5 and  $\rho_T^H$  is the thermal state of the system with respect to the Hamiltonian  $H$  and  $Z_H$  is the partition function. However, it has been further established that these restrictions are necessary but not sufficient in quantum thermodynamics as it deals with incoherent states only [33]. When the states possess coherence in energy eigenbasis then the transformation laws are more stringent than

this. In the presence of coherence, additionally the following constraint needs to be satisfied [33]

$$\Delta A_\alpha \leq 0, \quad \forall \alpha \geq 0. \quad (2.23)$$

Here,

$$\begin{aligned} A_\alpha(\rho) &= S_\alpha^R(\rho || \Delta_H(\rho)), \quad \text{when } \alpha \in [0, 1), \\ &= \tilde{S}_\alpha^R(\rho || \Delta_H(\rho)), \quad \text{when } \alpha \geq 1, \end{aligned} \quad (2.24)$$

where  $\Delta_H$  is the dephasing operation in the basis of Hamiltonian. Similar results have also been established following different approaches in Ref. [104]. Therefore, coherence put an additional restriction beyond free energy constraints in transforming quantum states under thermal operations.

### 2.5.1.2 Extracting work from coherence

Extracting work from quantum states is an important aspect of quantum thermodynamics as this constitutes the efficiency of thermal machines. Moreover, extracting work from quantum states is interesting to study as this can be useful in efficiently storing work in a quantum state. Extracting work by unitary operation is an active area of research. It has direct applications in the adiabatic work extraction in quantum thermal machines. A state from which no work can be extracted in a Hamiltonian process, in which the system returns to its initial Hamiltonian, is called passive state [105]. Such a process can be realized by unitary operation and the maximal extracted work in this process, ergotropy namely [106], is given by

$$W_{max}(\rho) = \max_U \text{Tr}[H(\rho - U\rho U^\dagger)]. \quad (2.25)$$

In other words, a state is passive if its average energy cannot be lowered by unitary operations. A passive state may not be completely passive [105], i.e., there exist examples where one cannot lower the average energy of  $n$  copies of a state, but can do the same of  $n + 1$  copies of the state. A state is called completely passive if no work can be extracted by unitary operations even when arbitrary large number of copies are used. It can be shown that only thermal states are completely passive [105, 107].

As work extraction is a fundamental aspect in quantum thermodynamics it is always interesting to enquire how much work can be extracted from coherence. Though coherence contributes to the free energy of a quantum state it cannot be converted to work directly. This is referred as work locking [33, 103, 108]. Due to work lock-

ing the analysis of Szilard that information is a source of work gets modified in the quantum domain [33]. However, coherence activation of work is possible which implies that work can be extracted from a coherent state in the presence of another coherent state. Extraction of work has been addressed in great detail in Ref. [109]. Further results on extracting work from coherence have been reported in Ref. [110]. Though we cannot extract work from quantum coherence, creating coherence has energy cost energy as we will see in chapter 3. This sheds light on the origin of irreversibility in quantum thermodynamics. Moreover, it is interesting to point out that work must be invested to maintain coherence of a quantum state in a thermal environment [111].

### 2.5.1.3 Quantum phase transitions

Coherence has been successfully employed to detect quantum phase transitions in anisotropic spin- $\frac{1}{2}$   $XY$  chain in a transverse magnetic field [112, 113]. It has also been shown that single spin based skew-information can detect quantum critical point as well as  $SU(2)$  symmetry point in  $XXZ$ – Heisenberg chains [114]. Utility of coherence quantifiers to detect quantum critical points in fermionic spin models has been reported recently [115, 116].

### 2.5.1.4 Quantum thermal machine

In Ref. [117], it has been demonstrated that if the initial qubits of a three qubit refrigerator possess even a little amount of coherence in energy eigenbasis then the cooling can be significantly better. The operation of a heat engine based on a driven three-level working fluid is shown to be better in the presence of coherence of the working fluid [42]. However, in contrary, it has been pointed out that quantum coherence may be detrimental to the speed of a minimal heat engine model based on a periodically modulated qubit [118], hybrid (of continuous and reciprocating) cycle heat engine [119]. This suggests that quantum coherence is at best optional for thermal machines and it requires further study to unravel potential role of coherence in the performance of thermal machines.

## 2.5.2 Other applications

It has been found that coherence plays important role and can be considered as a resource in various quantum technologies [57] including metrology [88], interference

phenomenon [63], quantum biological systems and transport phenomenon [92], quantum algorithms [120, 121], witnessing quantum correlations [77, 122], discriminating quantum channels [101, 102].

## 2.6 Chapter summary

In this chapter, we have studied the resource theory of quantum coherence identifying the free states and free operations, the incoherent states and incoherent operations namely. Next, we have discussed the criterion for a bona-fide coherence quantifier and established that relative entropy of coherence is a good measure of coherence which enjoys several operational and thermodynamic interpretations. Moreover, it can be computed easily for an arbitrary quantum state. We will use the relative entropy of coherence as a coherence quantifier to establish the thermodynamic cost of creating coherence in the next chapter. Further, we have also studied the applications of quantum coherence as a resource in thermodynamics and quantum technologies. We have seen that the description of quantum coherence in thermodynamic processes requires constraints beyond free energies. We have also seen that coherence cannot be used to extract work without activation which signifies the origin of irreversibility in quantum thermodynamics as we will see in the next chapter that one must spend energy to create coherence starting from a thermal environment.

# Thermodynamic cost of creating coherence

## 3.1 Introduction

In the previous two chapters, we have seen that considering the technological advancements towards processing of small scale quantum systems and proposals of nano-scale heat engines, it is of great importance to investigate the thermodynamic perspectives of quantum features like coherence and entanglement [19, 20, 57, 109, 110, 123, 124, 125, 126, 127, 128, 129, 130, 131, 132, 133, 134, 135]. Since energy conservation restricts the thermodynamic processing of coherence, a quantum state having coherence can be viewed as a resource in thermodynamics as it allows transformations that are otherwise impossible [32, 33]. In the last chapter, we have discussed the work extraction from quantum states, specially extractable work on the average by unitary operations or the ergotropy of the quantum states [105, 106]. We have also discussed that though coherence cannot always be converted into work, it is required to invest work to create coherence. Considering the huge number of applications of coherence in quantum thermodynamics and other quantum technological domains, it is of practical importance to investigate how one can create coherence with minimal thermodynamic resources.

With aforesaid motivation, we explore the intimate connections between the resource theory of quantum coherence and thermodynamic limitations on the processing of quantum coherence. Besides the work extraction by unitary transformations or ergotropy [106], it is also interesting to explore how much work has to be done to create quantum resources like coherence, entanglement by unitary operations starting from a thermal state. In this chapter, we study creating coherence by unitary operations with and without energy constraint. We go on even further to present a compara-

tive investigation of creation of quantum coherence and mutual information within the imposed thermodynamic constraints. Considering a thermally isolated quantum system initially in a thermal state, we perform an arbitrary unitary operation on the system to create coherence in energy eigenbasis. But before we discuss the results, let us digress on the importance of creating coherence in energy eigenbasis starting from a thermal state. Coherence in energy eigenbasis plays a crucial role in quantum thermodynamic protocols and several quantum information processing tasks. For example in Ref. [117], it has been demonstrated that if the initial qubits of a three qubit refrigerator possess even a little amount of coherence in energy eigenbasis then the cooling can be significantly better. In the small scale refrigerators, the three constituent qubits initially remain in corresponding thermal states associated with the three thermal baths. Therefore, one needs to create coherence by external means. Hence, creation of coherence from thermal states may be fruitful and far-reaching for better functioning of various nano scale thermal machines and various thermodynamic protocols. These are the main motivations for studying creation of coherence from thermodynamic perspective. We consider closed quantum systems and hence allow only unitary operations for creating coherence. Of course, after creating the coherence via the unitary transformation we have to isolate or take away the system from the heat bath so that it does not get thermalized again.

In this chapter, first we find the upper bound on the coherence that can be created using arbitrary unitary operations starting from a fixed thermal state and then we show explicitly that irrespective of the temperature of the initial thermal state the upper bound on coherence can always be saturated. Such a physical process will cost us some amount of energy and hence it is natural to ask that if we have a limited supply of energy to invest then what is the maximal achievable coherence in such situations? Further, we investigate whether both coherence and mutual information can be created maximally by applying a single unitary operation on a two qubit quantum system. We find that it is not possible to achieve maximal quantum coherence and mutual information simultaneously. Our results are relevant for the quantum information processing in physical systems where thermodynamic considerations cannot be ignored as we have discussed in the preceding paragraph.

## 3.2 Maximum achievable coherence under arbitrary unitary operations

Let us now consider the creation of maximal coherence in energy eigenbasis, which we define shortly, starting from a thermal state by unitary operations. The prime motivation for starting with a thermal initial state is that the surrounding may be considered as a thermal bath and as the system interacts with the surrounding, it eventually gets thermalized. However, our protocol for creating maximal coherence is applicable for any incoherent state. Let us now consider an arbitrary quantum system in contact with a heat bath at temperature  $T = 1/\beta$ . The thermal state of a system with Hamiltonian  $H = \sum_{j=0}^{d-1} E_j |j\rangle \langle j|$  is given by

$$\rho_T = \frac{1}{Z} e^{-\beta H}, \quad (3.1)$$

where  $d$  is the dimension of the Hilbert space and  $Z = \text{Tr}[e^{-\beta H}]$  is the partition function. The maximum amount of coherence  $C_{r,max}(\rho_f)$  that can be created starting from  $\rho_T$  by unitary operations is given by

$$C_{r,max}(\rho_f) = \max_{\{\rho_f | S(\rho_f) = S(\rho_T)\}} \{S(\rho_f^D) - S(\rho_f)\}. \quad (3.2)$$

As the maximum entropy of a quantum state in  $d$ -dimension is  $\log d$ , the amount of coherence that can be created starting from  $\rho_T$ , by a unitary transformation, always follows the inequality

$$C_r(\rho_f) \leq \log d - S(\rho_T). \quad (3.3)$$

Now the question is whether the bound is tight or not, i.e., is there any unitary operation that can lead to the creation of  $\log d - S(\rho_T)$  amount of coherence starting from  $\rho_T$ ? We show that the bound in Eq. (3.3) is achievable by finding the unitary operation  $U$  such that  $\rho_f = U\rho_i U^\dagger$  has maximal amount of coherence. Since the relative entropy of coherence of  $\rho_f$  is given by  $S(\rho_f^D) - S(\rho_f)$ , one has to maximize the entropy of the diagonal density matrix  $\rho_f^D$ . The quantum state that is the diagonal of a quantum state  $\rho$  is denoted as  $\rho^D$  throughout the chapter.

First, we construct a unitary transformation that results in rotating the energy eigenbasis to the maximally coherent basis as follows. The maximally coherent basis

$\{|\phi_j\rangle\}_j$  is defined as  $|\phi_j\rangle = \mathbb{Z}^j |\phi\rangle$ , where

$$\mathbb{Z} = \sum_{m=0}^{d-1} e^{\frac{2\pi im}{d}} |m\rangle \langle m|, \quad (3.4)$$

and  $|\phi\rangle = \frac{1}{\sqrt{d}} \sum_{i=0}^{d-1} |i\rangle$ . It can be verified easily that,  $\langle \phi_j | \phi_k \rangle = \delta_{jk}$ . Also, note that all the states in  $\{|\phi_j\rangle\}_j$  and  $|\phi\rangle$  are the maximally coherent states [59] and have equal amount of the relative entropy of coherence which is equal to  $\log d$ . Now consider the unitary operation

$$U = \sum_j |\phi_j\rangle \langle j|, \quad (3.5)$$

which changes energy eigenstate  $|j\rangle$  to the maximally coherent state  $|\phi_j\rangle$ . Starting from the thermal state  $\rho_T$ , the final state  $\rho_f$  after the application of  $U$  is given by

$$\rho_f = \sum_j \frac{e^{-\beta E_j}}{Z} |\phi_j\rangle \langle \phi_j|. \quad (3.6)$$

Since  $\rho_f$  is a mixture of pure states that all have maximally mixed diagonals, the bound in Eq. (3.3) is achieved. We note that  $U$  in Eq. (3.5) is only one possible choice among the possible unitaries achieving the bound in Eq. (3.3). For example, any permutation of the indices  $j$  of  $|\phi_j\rangle$  in Eq. (3.5) is also a valid choice to achieve the bound. It is worth mentioning that even though we consider thermal density matrix to start with to create maximal coherence in energy eigenbasis, following the same protocol maximal coherence can be created from any arbitrary incoherent state in any arbitrary reference basis.

To create coherence by unitary operations starting from a thermal state, some amount of energy is required. Now, let us ask how much energy is needed on an average to create the maximal amount of coherence. Let  $\rho_T \rightarrow V\rho_T V^\dagger$ , then the energy cost of any arbitrary unitary operation  $V$  acting on the thermal state is given by

$$W = \text{Tr}[H(V\rho_T V^\dagger - \rho_T)]. \quad (3.7)$$

Since we are dealing with energy eigenbasis, we have  $E(\rho^D) = E(\rho)$ . Here  $E(\rho) = \text{Tr}(H\rho)$  is the average energy of the system in the state  $\rho$ . The energy cost to create

maximum coherence given in Eq. 3.3, starting from the thermal state  $\rho_T$  is given by

$$W_{max} = \text{Tr}[H(U\rho_T U^\dagger - \rho_T)] = \frac{1}{d}\text{Tr}[H] - \frac{1}{Z}\text{Tr}[H e^{-\beta H}]. \quad (3.8)$$

Here  $U$  is given by Eq. (3.5). Note that maximal coherence can always be created by unitary operations starting from a finite dimensional thermal state at an arbitrary finite temperature, with finite energy cost. However, it is not possible to create coherence by unitary operation starting from a thermal state at infinite temperature i.e., the maximally mixed state.

### 3.3 Creating coherence with limited energy

Since energy is an independent resource, it is natural to consider a scenario where creation of coherence is limited by a constraint on available energy. In this section we consider creation of optimal amount of coherence at a limited energy cost  $\Delta E$  starting from  $\rho_T$ . To maximize the coherence, one needs to find a final state  $\rho_f$  whose diagonal part  $\rho_f^D$  has maximum entropy with fixed average energy  $E_T + \Delta E$ , where  $E_T$  is the average energy of the initial thermal state  $\rho_T$ . Note that  $E(\rho_f^D) = E(\rho_f)$ . From maximum entropy principle [17, 18], we know that the thermal state has maximum entropy among all states with fixed average energy. Therefore, the maximum coherence  $C_{r,max}^{\Delta E}$  that can be created with  $\Delta E$  amount of available energy is upper bounded by

$$C_{r,max}^{\Delta E} \leq S(\rho_{T'}) - S(\rho_T). \quad (3.9)$$

Here  $\rho_{T'}$  is a thermal state at a higher temperature  $T'$  such that  $\Delta E = \text{Tr}[H(\rho_{T'} - \rho_T)]$ . Thus, in order to create maximal coherence at a limited energy cost, one should look for a protocol such that the diagonal part of  $\rho_f$  is a thermal state at a higher temperature  $T'$  (depending on the energy spent  $\Delta E$ ), i.e.,  $\rho_f^D = \rho_{T'}$ . Now it is obvious to inquire whether there always exists an optimal unitary  $U^{opt}$  that serves the purpose. Theorem 1 answers this question in affirmative.

**Theorem 1** *There always exists a real orthogonal transformation  $R$  that creates maximum coherence  $S(\rho_{T'}) - S(\rho_T)$ , starting from the thermal state  $\rho_T$  and spending only  $\Delta E = \text{Tr}[H(\rho_{T'} - \rho_T)]$  amount of energy.*

Before going to the proof of the theorem let us define a few terms that will be used

in proving the theorem.

- *Doubly stochastic matrix:* A  $d \times d$  matrix  $M = (M_{ab})$  ( $a \in \{1, \dots, d\}$ ,  $b \in \{1, \dots, d\}$  and  $M_{ab} \geq 0$ ) is called a doubly stochastic matrix if  $\sum_a M_{ab} = 1$  for all  $b$  and  $\sum_b M_{ab} = 1$  for all  $a$  [136].
- *Unitarystochastic matrix:* Consider a  $d \times d$  unitary matrix  $U = (U_{ab})$  ( $a \in \{1, \dots, d\}$ ,  $b \in \{1, \dots, d\}$ ) such that  $U^\dagger U = \mathbb{I}$ . Here, superscript  $\dagger$  denotes the conjugate transpose and  $\mathbb{I}$  is a  $d \times d$  identity matrix. The matrix  $(|U_{ab}|^2)$  forms a doubly stochastic matrix and such a matrix is called unitarystochastic matrix [136].
- *Orthostochastic matrix:* Consider a  $d \times d$  real orthogonal matrix  $O = (O_{ab})$  ( $a \in \{1, \dots, d\}$ ,  $b \in \{1, \dots, d\}$ ) such that  $O^T O = \mathbb{I}$ . Here, superscript  $T$  denotes the transpose and  $\mathbb{I}$  is a  $d \times d$  identity matrix. The matrix  $(O_{ab}^2)$  forms a doubly stochastic matrix and such a matrix is called orthostochastic matrix [136].
- *Majorization:* Let  $\vec{x}$  and  $\vec{y}$  be two normalized probability vectors with equal dimension say  $d$ , then we say  $\vec{x}$  majorizes  $\vec{y}$ , and denote by  $\vec{y} \prec \vec{x}$  if

$$\sum_{i=1}^k x_i^\downarrow \geq \sum_{i=1}^k y_i^\downarrow, \quad 1 \leq k \leq d, \quad (3.10)$$

where  $\downarrow$  denotes that the entries are in decreasing order. Moreover,  $\vec{y} \prec \vec{x}$  iff  $\vec{y} = D\vec{x}$  for some doubly stochastic matrix  $D$  [136].

**Proof 1** *To prove the theorem, we first show that the unitary transformations on a quantum state induce doubly stochastic maps on the diagonal part of the quantum state. Note that, we start from the thermal state  $\rho_T = \sum_{j=0}^{d-1} \frac{e^{-\beta E_j}}{Z} |j\rangle \langle j|$ . The diagonal part of  $\rho_T$  transforms under the action of a unitary  $U$  as follows:*

$$\text{diag}\{U\rho_T U^\dagger\} = \sum_{i=0}^{d-1} q_i |i\rangle \langle i|,$$

where  $q_i = \frac{1}{Z} \sum_{j=0}^{d-1} M_{ij} e^{-\beta E_j}$  and  $M$ , with entries  $M_{ij} = \langle i|U|j\rangle \langle j|U^\dagger|i\rangle$ , is a doubly stochastic matrix. Therefore, the diagonal part is transformed by the doubly-stochastic matrix  $M$  such that

$$\vec{Q} = M\vec{P}_T,$$

where  $\vec{P}_T = \frac{1}{Z} \{e^{-\beta E_0}, e^{-\beta E_1}, \dots, e^{-\beta E_{d-1}}\}^T$  is the diagonal vector corresponding to the initial thermal state  $\rho_T$  and  $\vec{Q}$  is the diagonal vector corresponding to the final state.

For two thermal states  $\rho_{T''}$  and  $\rho_T$ , corresponding to the same Hamiltonian, we have  $\vec{P}_{T''} \prec \vec{P}_T$  if  $T'' > T$  [137], where  $\vec{P}_{T''}$  and  $\vec{P}_T$  are the diagonal vectors of  $\rho_{T''}$  and  $\rho_T$  respectively. From the results of the theory of majorization [136], it follows that there always exists an orthostochastic matrix  $B'$  such that  $\vec{P}_{T''} = B' \vec{P}_T$ .

Note that the diagonal vectors corresponding to the thermal states  $\rho_{T'}$  and  $\rho_T$  in Eq.3.9 always satisfy  $\vec{P}_{T'} \prec \vec{P}_T$  as  $\Delta E \geq 0$ . Therefore, there always exist an orthostochastic matrix  $B$  such that

$$\vec{P}_{T'} = B \vec{P}_T. \quad (3.11)$$

Let  $R$  be a real orthogonal operator corresponding to the orthostochastic matrix  $B$  in Eq.3.11. Then,  $R$  transform the initial thermal state  $\rho_T$  to a final state  $\rho_f$  such that  $\rho_f^D = \rho_{T'}$ . Therefore, there always exists a real orthogonal transformation  $R$  that creates  $S(\rho_{T'}) - S(\rho_T)$  amount of coherence, starting from the thermal state  $\rho_T$  and spending only  $\Delta E = \text{Tr}[H(\rho_{T'} - \rho_T)]$  amount of energy. This completes the proof.

### 3.3.1 Example: Qubit system

In the following, we find out explicitly the real unitary transformation that allows creation of maximal coherence with limited energy at our disposal for the case of a qubit system with the Hamiltonian  $H = E|1\rangle\langle 1|$ . The initial thermal state is given by  $\rho_T = p|0\rangle\langle 0| + (1-p)|1\rangle\langle 1|$  with  $p = \frac{1}{1+e^{-\beta E}}$ . Now our goal is to create maximal coherence by applying an optimal unitary  $U^*$ , investing only  $\Delta E$  amount of energy. The average energy of the initial thermal state  $\rho_T$  is given by  $(1-p)E$ . As we have discussed earlier that for maximal coherence creation with  $\Delta E$  energy cost, the diagonal part of the final state must have to be a thermal state,  $\rho_{T'} = q|0\rangle\langle 0| + (1-q)|1\rangle\langle 1|$ , at some higher temperature  $T'$ , with average energy  $(1-p)E + \Delta E$ . Here,  $q$ , and hence  $T'$ , is determined from the energy constraint as  $q = p - \frac{\Delta E}{E} = \frac{1}{1+e^{-\beta' E}}$ . From theorem 1, it is evident that there always exists a rotation operator  $R$  which creates the maximal coherence. Consider a rotation operator of the form

$$R(\theta) = \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix} \quad (3.12)$$

that transforms  $\rho_T$  as follows

$$\begin{aligned}\rho_f &= R(\theta)\rho_T R^T(\theta) \\ &= \begin{pmatrix} p \cos^2 \theta + (1-p) \sin^2 \theta & (2p-1) \sin \theta \cos \theta \\ (2p-1) \sin \theta \cos \theta & p \sin^2 \theta + (1-p) \cos^2 \theta \end{pmatrix}.\end{aligned}$$

We need the diagonal part of the final state to be the thermal state  $\rho_{T'}$  at a higher temperature  $T'$ . Therefore,

$$q = p \cos^2 \theta + (1-p) \sin^2 \theta. \quad (3.13)$$

As R.H.S of Eq. (3.13) is a convex combination of  $p$  and  $(1-p)$  and  $p \geq q \geq 1/2 \geq (1-p)$ , by suitably choosing  $\theta$  we can reach to the desired final state  $\rho_f$  such that  $\rho_f^D = \rho_{T'}$ . The angle of rotation  $\theta$  is given by

$$\theta = \cos^{-1} \left( \sqrt{\frac{p+q-1}{2p-1}} \right). \quad (3.14)$$

Thus, the maximal coherence at constrained energy cost  $\Delta E$  can be created from a qubit thermal state by a two dimensional rotation operator as given by Eq. (3.12).

### 3.3.2 Example: Qutrit system

For qubit systems, a two dimensional rotation with the suitably chosen  $\theta$  is required to create maximum coherence starting from a thermal state at a finite temperature with limited available energy. For higher dimensional systems, it follows from theorem 1, that there always exists a rotation which serves the purpose of maximal coherence creation. However, finding the exact rotation operator for a given initial thermal density matrix and energy constraint is not an easy task. Even for a qutrit system finding the optimal rotation is nontrivial. In what follows, we demonstrate the protocol for creating maximal coherence with energy constraint starting from a thermal state for qutrit systems. Note that by applying a unitary operation on a thermal qubit, one has to invest some energy and thus, the excited state population corresponding to diagonal part of the final qubit is always increased. Therefore, for the case of qubit systems, one only has to give a rotation by an angle  $\theta$ , depending on the available energy to create maximal coherence starting from a given thermal state. For a thermal state in higher dimension, we know that with the increment in temperature (energy), the occupation probability of the ground state will always

decrease and the occupation probability will increase for the highest excited state. But what will happen for the intermediate energy levels? Let us first answer this particular question considering an initial thermal state of the form

$$\rho_T = \sum_{j=0}^{d-1} p_j |j\rangle\langle j|, \quad (3.15)$$

where  $p_j = \frac{e^{-E_j/T}}{\sum_j e^{-E_j/T}}$  is the occupation probability of the  $j^{\text{th}}$  energy level. Differentiating  $p_j$  with respect to the temperature, we get

$$\frac{\partial p_j}{\partial T} = -\frac{(\langle E \rangle_T - E_j)}{T^2} p_j. \quad (3.16)$$

Therefore, for energy levels lying below the average energy of the thermal state, the occupation probabilities will decrease with the increase of temperature and the occupation probabilities will increase for the energy levels lying above the average energy. Making use of this change in occupation probabilities, we now provide a protocol for maximum coherence creation in thermal qutrit systems with a constraint on the available energy. We consider a qutrit system with the system Hamiltonian  $H = E|1\rangle\langle 1| + 2E|2\rangle\langle 2|$ . The initial thermal qutrit state is given by  $\rho_T = p|0\rangle\langle 0| + (1 - p - q)|1\rangle\langle 1| + q|2\rangle\langle 2|$  with average energy  $\langle E \rangle_T = (1 - p - q)E + 2qE$ . Here  $p = 1/Z$  and  $q = e^{-2\beta E}/Z$ , where  $Z = 1 + e^{-\beta E} + e^{-2\beta E}$  is the partition function. The diagonal density matrix of the final state is a thermal qutrit state at temperature  $T'$  with average energy  $\langle E \rangle_{T'} = (1 - p - q)E + 2qE + \Delta E$ , when we create coherence with  $\Delta E$  energy constraint.

We show that just two successive rotations in two dimensions is sufficient for maximum coherence creation. For equal energy spacing of  $\{0, E, 2E\}$ , the average energy at infinite temperature is given by  $\langle E \rangle_\infty = E$ . So, for an arbitrary finite temperature, the condition  $E > \langle E \rangle_T$  holds true. Thus for the aforementioned qutrit thermal system, with the increase in temperature, the occupation probabilities of the first and second excited states will always increase at the expense of the decrease in occupation probability for the ground state. The diagonal elements of the final state should be the occupation probabilities of the thermal state at a higher temperature  $T'$ , given by  $p', 1 - p' - q'$  and  $q'$  for the ground, first and second excited states,

respectively. From the conservation of probabilities, it follows that

$$\begin{aligned} -\Delta p = p - p' &= (q' - q) + (1 - p' - q') - (1 - p - q) \\ &= \Delta q + \Delta(1 - p - q), \end{aligned} \quad (3.17)$$

Note that, we always have  $-\Delta p > \Delta q > 0$ .

Now, let us first apply a rotation about  $|1\rangle$ . Physically, this rotation creates coherence between basis states  $|0\rangle$  and  $|2\rangle$ . The rotation can be expressed by the unitary  $R_1(\alpha) = e^{-i\alpha J_1}$ , where

$$J_1 = \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix} \quad (3.18)$$

is the generator of the rotation. Then another rotation is applied about  $|2\rangle$ , which is given by  $R_2(\delta) = e^{-i\delta J_2}$ , where

$$J_2 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \quad (3.19)$$

After the action of two successive rotations, given by  $R_2(\delta)R_1(\alpha)$ , we have

$$q' = q \cos^2 \alpha + p \sin^2 \alpha \quad (3.20)$$

and

$$\begin{aligned} p' &= (q \sin^2 \alpha + p \cos^2 \alpha) \cos^2 \delta + (1 - p - q) \sin^2 \delta \\ &= (p - \Delta q) \cos^2 \delta + (1 - p - q) \sin^2 \delta. \end{aligned} \quad (3.21)$$

From Eq. (3.20), it is clear that  $q'$  is a convex combination of  $p$  and  $q$ , and since  $q < q' < p$ , there always exists a angle of rotation  $\alpha$ , depending on the available energy so that the protocol can be realized. The angle of rotation is given by  $\alpha = \cos^{-1} \sqrt{\frac{p-q'}{p-q}}$ , where  $\alpha \in [0, \pi/2]$ . Similarly, Eq. (3.21), suggests that  $p'$  is a convex combination of  $(p - \Delta q)$  and  $(1 - p - q)$  and since  $1 - p - q < p' < p - \Delta q$  (Eq.3.17), one can always achieve any desired value of  $p'$ , by suitably choosing  $\delta \in [0, \pi/2]$ , with  $\delta = \cos^{-1} \sqrt{\frac{p'-(1-p-q)}{(p-\Delta q)-(1-p-q)}}$ . Thus, maximal coherence at finite energy cost can

be created by two successive two dimensional rotations starting from a thermal state of a qutrit system. Note that we have considered equal energy spacing  $\{0, E, 2E\}$ , however, the above protocol will hold for any energy spacing for which the condition  $E_1 > \langle E \rangle_T$  holds, where  $E_1$  is the energy of the energy eigenstate  $|1\rangle$ .

### 3.4 Energy cost of preparation: Coherence versus correlation

In this section we carry out a comparative study between maximal coherence creation and maximal total correlation creation (also see Ref. [133]) with limited available energy. We consider an arbitrary  $N$  party system acting on a Hilbert space  $\mathcal{H}^{d_1} \otimes \mathcal{H}^{d_2} \otimes \dots \otimes \mathcal{H}^{d_N}$ . The Hamiltonian of the composite system is non-interacting and given by  $H_{tot} = H_1 + H_2 + \dots + H_N$ . For the sake of simplicity we consider  $H_1 = H_2 = \dots = H_N = H$ . However, our results hold in general. Suppose there exists an optimal unitary operator  $U^{opt}$  which creates maximal total correlation from initial thermal state  $\rho_T$  with  $\Delta E$  energy cost. It is shown in Ref. [133] that the maximal correlation (multipartite mutual information) that can be created by a unitary transformation with energy cost  $\Delta E$  is given by

$$I_{max}^{\Delta E} = \sum_i [S(\rho_{T'}^i) - S(\rho_T^i)], \quad (3.22)$$

where  $\rho_T^i$  denotes the thermal state of the  $i$ th marginal at temperature  $T$ . Note that as the systems are non-interacting the global thermal state is the product of the local thermal states. Clearly,  $T'$  is greater than  $T$  and  $T'$  can be determined from the amount of available energy  $\Delta E$ . The definition of the total correlation or the multipartite mutual information considered in [133] is similar to the one we use in chapter 4 in Eq 4.14, for bipartite states which can be defined for multipartite scenario also. In the protocol to achieve the maximal correlation, the subsystems of the composite system  $\rho_T^N$  transform to the thermal states  $\rho_{T'}^i$  of the corresponding individual systems at some higher temperature  $T'$  [133]. It is interesting to inquire that how much coherence is created during this process as in several quantum information processing tasks it may be needed to create both the coherence and correlation, simultaneously. The amount of coherence created  $C_r|_{I_{max}^{\Delta E}}$ , when the unitary transformation creates

maximal correlation is given by

$$C_r|_{I_{max}^{\Delta E}} = S(\rho_f^D) - \sum_i S(\rho_T^i). \quad (3.23)$$

As the Hamiltonian is noninteracting,  $\rho_f^D$  and the product of the marginals ( $\prod^{\otimes i} \rho_{T'}^i$ ) have the same average energy. Since the product of the marginals is the thermal state of the composite system at temperature  $T'$ , the maximum entropy principle implies that  $\sum_i S(\rho_{T'}^i) \geq S(\rho_f^D)$ . Hence,  $C_r|_{I_{max}^{\Delta E}} \leq I_{max}^{\Delta E}$ . Therefore, when one aims for maximal correlation creation the coherence created is always bounded by the amount of correlation created. Now, we ask the converse, i.e., how much correlation can be created when one creates maximal coherence by a unitary operation with the same energy constraint  $\Delta E$ ? The maximal coherence that can be created in this scenario by unitary transformation with energy constraint is given by

$$C_{r,max}^{\Delta E} = \sum_i [S(\rho_{T'}^i) - S(\rho_T^i)]. \quad (3.24)$$

Note that the maximal achievable coherence is equal to the maximal achievable correlation (cf. Eq. (3.22)), but the protocols to achieve them are completely different. When the maximal coherence is created, the diagonal of the final density matrix is a thermal state at some higher temperature while the maximal correlation is created when the product of the marginals of the final state is a thermal state at some higher temperature. Therefore, when the maximum amount of coherence  $C_{r,max}^{\Delta E}$  is created, the correlation  $I|_{C_{r,max}^{\Delta E}}$  that is created simultaneously always satisfies

$$I|_{C_{r,max}^{\Delta E}} \leq C_{r,max}^{\Delta E}. \quad (3.25)$$

The above equation again follows from the maximum entropy principle and the fact that the diagonal part and the product of the marginals have same average energy. Therefore, when one aims for maximal coherence creation, the amount of correlation that can be created at the same time is always bounded by the maximal coherence created and vice versa.

### 3.4.1 Simultaneous creation of maximal coherence and correlation

It is also interesting to inquire whether one can create maximal coherence and correlation simultaneously. In the following, we partially answer this question. For two qubit systems we show that there does not exist any unitary which maximizes both the coherence and correlation, simultaneously. Let the Hamiltonian of the two qubit system be given by  $H_{AB} = H_A + H_B$  with  $H_A \neq H_B$ , in general. Later, we also consider  $H_A = H_B$ . The initial state is the thermal state at temperature  $T$  and given by

$$\rho_{AB,T} = \text{diag}\{pq, p(1-q), (1-p)q, (1-p)(1-q)\}, \quad (3.26)$$

where  $p = 1/(1 + e^{-\beta E_A})$ ,  $q = 1/(1 + e^{-\beta E_B})$ ,  $H_A = E_A|1\rangle\langle 1|$  and  $H_B = E_B|1\rangle\langle 1|$ . Consider the protocol of Ref. [133] to create the maximum correlation. In that scenario, the marginals are the thermal states at a higher temperature  $T'$ . Let the final state of the two qubit system after the unitary transformation is given by

$$\rho_{AB}^f = \sum_{ijkl} a_{ijkl} |i\rangle\langle j| \otimes |k\rangle\langle l|. \quad (3.27)$$

As the marginals are thermal,  $a_{iikl} = 0$  if  $k \neq l$  and  $a_{ijkk} = 0$  if  $i \neq j$ . Thus, the maximally correlated state that is created by investing a limited amount of energy is an  $X$ -state. The  $X$ -states are a special class of states that have been analyzed in great detail in context of analytical calculations of quantum discord [138, 139] among others. The term  $X$ -states has been coined in Ref. [140] for their visual appearance. For bipartite qubit quantum systems, the states  $\rho_X$  of the form

$$\rho_X := \begin{pmatrix} \rho_{00} & 0 & 0 & \rho_{03} \\ 0 & \rho_{11} & \rho_{12} & 0 \\ 0 & \rho_{21} & \rho_{22} & 0 \\ \rho_{30} & 0 & 0 & \rho_{33} \end{pmatrix}$$

are called  $X$ -states. In general, any density matrix that has nonzero elements only at the diagonals and anti-diagonals is called an  $X$ -state. For a detailed exposition of  $X$ -states see Ref. [141]. While for maximal coherence creation, the diagonal part of the final state is a thermal state at higher temperature  $T'$ . Therefore, the diagonal

part of the final state must be of the form

$$\rho_{AB,T'}^{fD} = \text{diag}\{p'q', p'(1-q'), (1-p')q', (1-p')(1-q')\},$$

where  $p' = 1/(1 + e^{-\beta'E_A})$ ,  $q' = 1/(1 + e^{-\beta'E_B})$ ,  $p' < p$  and  $q' < q$  as  $\beta' < \beta$ . We show separately for (i)  $E_A = E_B$  and (ii)  $E_A \neq E_B$ , that there is no such unitary transformation which serves the purpose. It will be interesting to explore what happens for higher dimensional systems.

**(i)  $\mathbf{E}_A = \mathbf{E}_B$ :**

For the case where the initial state is  $\rho_T^{\otimes 2}$  with  $\rho_T = \rho_T^A = \rho_T^B = \text{diag}\{p, 1-p\}$  and the final state is in the  $X$ -state form, given by

$$\rho_f = \begin{pmatrix} q^2 & 0 & 0 & Y \\ 0 & q(1-q) & X & 0 \\ 0 & X^* & q(1-q) & 0 \\ Y^* & 0 & 0 & (1-q)^2 \end{pmatrix}. \quad (3.28)$$

Note that  $p \geq q \geq 1/2 \geq (1-q) \geq (1-p)$ . Here,  $|Y| \leq q(1-q)$  and  $|X| \leq q(1-q)$  so that,  $\rho_f$  is positive semi-definite. Let  $p = \frac{1}{2} + \epsilon$  and  $q = \frac{1}{2} + \epsilon'$ , where  $\frac{1}{2} > \epsilon > \epsilon' > 0$ . The eigenvalues of this final density matrix are given by

$$\lambda_{1,4} = \frac{1}{2} \left( q^2 + (1-q)^2 \pm \sqrt{(q^2 - (1-q)^2)^2 + 4|Y|^2} \right), \quad (3.29)$$

$$\lambda_{2,3} = q(1-q) \pm |X|. \quad (3.30)$$

As the unitary transformation preserves the eigenvalues, two of the eigenvalues of the final density matrix must be equal to  $p(1-p)$  and the other two must be equal to  $p^2$  and  $(1-p)^2$  respectively. In the following we show that this is not possible.

**Case (1):** Let us first assume  $\lambda_2 = \lambda_3 = p(1-p)$ . Then we find that  $|X| = 0$  and  $q = p$  or  $q = 1-p$ . Since we know  $p \geq 1/2$ , then  $q \leq 1/2$  for  $q = 1-p$ . Hence,  $q \neq 1-p$ .  $q = p$  can only happen under identity operation. Therefore,  $\lambda_2 \neq \lambda_3$ .

**Case 2:** Assume  $\lambda_1 = \lambda_4 = p(1-p)$ , then we have

$$\begin{aligned} p(1-p) &= \frac{q^2 + (1-q)^2}{2} + \frac{q^2 - (1-q)^2}{2} M \\ &= \frac{q^2 + (1-q)^2}{2} - \frac{q^2 - (1-q)^2}{2} M, \end{aligned} \quad (3.31)$$

where  $M = \sqrt{1 + \frac{4|Y|^2}{(2q-1)^2}}$ . From Eq. (3.31), we have  $M = 0$  which is a contradiction

since  $M \geq 1$ . Therefore, Eq. (3.31) cannot be satisfied.

**Case 3:** As  $p^2 \geq p(1-p) \geq (1-p)^2$ , other two possibilities are  $\lambda_1 = \lambda_3 = p(1-p)$  or  $\lambda_4 = \lambda_2 = p(1-p)$ . Note that we always have  $\lambda_1 > \lambda_3$ . Therefore, the only possibility we have to check is  $\lambda_4 = \lambda_2 = p(1-p)$ . For that we have

$$\begin{aligned} \lambda_2 = p(1-p) &\Rightarrow |X| = p(1-p) - q(1-q) \\ &\Rightarrow |X| = -(\epsilon^2 - \epsilon'^2), \end{aligned} \tag{3.32}$$

which is a contradiction as the R.H.S. is negative since  $\epsilon > \epsilon'$ . Therefore, it is also not possible.

(ii)  $\mathbf{E}_A \neq \mathbf{E}_B$ :

Let us relabel the diagonal entries of the initial density matrix as

$$\rho_T^{AB} = a_1|00\rangle\langle 00| + a_2|01\rangle\langle 01| + a_3|10\rangle\langle 10| + a_4|11\rangle\langle 11|.$$

Here,  $\{a_i\}$  is an arbitrary probability distribution that depends on the energy levels  $E_A, E_B$  and the initial temperature  $T$ . We argue that the unitary transformations that map the initial state into an  $X$ -state starting from a two qubit thermal state at arbitrary finite temperature  $T$ , are only allowed to create correlation among the subspaces spanned by  $\{|00\rangle, |11\rangle\}$  and  $\{|01\rangle, |10\rangle\}$ , separately, i.e., no correlation can be created between these two subspaces. Thus, the unitary transformation that maximizes the total correlation acts on the blocks spanned by  $\{|00\rangle, |11\rangle\}$  and  $\{|01\rangle, |10\rangle\}$ , separately. Given this, again from comparing eigenvalues, it can be argued that total correlation and coherence cannot be maximized simultaneously by unitary transformations in two qubit systems when the Hamiltonian of the systems are not the same.

## 3.5 Chapter summary

In this chapter, we have studied the creation of quantum coherence by unitary transformations starting from a thermal state. This is important from practical view point, as most of the systems interact with the environment and get thermalized eventually. We find the maximal amount of coherence that can be created from a thermal state at a given temperature and find a protocol to achieve this. Moreover, we find the amount of coherence that can be created with limited available energy. Thus, our study establishes a link between coherence and thermodynamic resource

theories and reveals the limitations imposed by thermodynamics on the processing of the coherence. Additionally, we have performed a comparative study between the coherence creation and total correlation creation with the same amount of energy at our disposal. We show that when one creates the maximum coherence with limited energy, the total correlation created in the process is always upper bounded by the amount of coherence created and vice versa. As correlation and coherence both are useful resources, processing them simultaneously is fruitful. However, our result shows that, at least in two qubit systems, there is no way to create the maximal coherence and correlation simultaneously via unitary transformations. Recently, the importance of coherence in improving the performance of thermal machines has been explicitly established and the implications of coherence on the thermodynamic behavior of quantum systems have been studied. Therefore, it is justified to believe that the study of the thermodynamic cost and limitations of thermodynamic laws on the processing of quantum coherence can be far reaching. The results in this chapter are a step forward in this direction.

**N.B.** The results of this chapter are original. We study creation of quantum coherence in energy eigenbasis starting from a thermal state with and without constraint on the available energy. We give a protocol to create maximum coherence when there is no limitation on energy. Furthermore, we show that there always exists a real unitary operation that creates maximum coherence with limited energy starting from a thermal state and construct protocols for two and three dimensions. We compare simultaneous creation of coherence and total correlation with limited energy and show that it is not possible to create maximum coherence and maximum total correlation simultaneously in two dimension. Creation of total correlation has been studied in Ref. [133] and we have used the result of this paper while comparing simultaneous creation of coherence and total correlation.

The results of this chapter have been published in “*Energy cost of creating quantum coherence*, A. Misra, U. Singh, S. Bhattacharya, A.K. Pati, *Phys. Rev. A*, **93**, 052335 (2016).”

# Quantum correlations

## 4.1 Introduction

Characterization and quantification of quantum correlation [12, 22] play a central role in quantum information. Entanglement, in particular, has been successfully identified as a useful resource for different quantum communication protocols and computational tasks [2, 3, 4, 5]. Moreover, it has also been employed to study cooperative quantum phenomena like quantum phase transitions in many-body systems [36, 37]. However, in the recent past, several quantum phenomena of shared systems have been discovered in which entanglement is either absent or does not play any significant role. Locally indistinguishable orthogonal product states [142, 143, 144, 145, 146] is a prominent example where entanglement does not play an important role. The role of entanglement is also unclear in the model of deterministic quantum computation with one quantum bit [147, 148]. Such phenomena motivated the search for concepts and measures of quantum correlation independent of the entanglement-separability paradigm. Introduction of quantum discord [138, 139] is one of the most important advancements in this direction and has inspired a lot of research activity [22]. It has thereby emerged that quantum correlations, independent of entanglement, can also be a useful ingredient in several quantum information processing tasks [22]. Other measures in the same direction include quantum work deficit [21, 149, 150], measurement-induced nonlocality [151], and quantum deficit [152, 153]. These measures can be generally considered to be quantum correlation measures within an “information-theoretic paradigm”. In what follows, we briefly review quantum entanglement and quantum correlations beyond entanglement.

## 4.2 Quantum entanglement

Characterization and quantification of quantum entanglement [12] lies at the heart of quantum information theory, since its early recognition as “spooky action at a distance” in the Einstein-Podolsky-Rosen article [154]. It has been successfully identified as a key resource in several quantum communication protocols including superdense coding [2], teleportation [3], and quantum cryptography [6, 7]. In the resource theory of entanglement [12], as distributing entanglement over the parties that are far apart is difficult due to loss of quantumness during the transport, all entangled states are considered as valuable resources. Thus, the states that are not entangled and the operation that cannot create entanglement are considered as free states and free operations. Any operation that can create entanglement between the shared quantum states are also considered as a resource.

### 4.2.1 Local operations classical communication

In QRT of entanglement, the free operations are the Local operations classical communication (LOCC). In a general LOCC protocol, the parties can act only locally and are allowed to communicate classically. However, by these LOCC no entanglement can be created among distant parties and therefore these are the class of free operations in the QRT of entanglement [12].

### 4.2.2 Separable states

A general quantum state shared by  $A$  and  $B$ , that can be prepared by LOCC between  $A$  and  $B$ , is of the form [155]

$$\rho_{AB} = \sum_{a=1}^k p \rho_A^a \otimes \rho_B^a, \quad (4.1)$$

where  $\rho_A^a$  and  $\rho_B^a$  are quantum states defined on local Hilbert spaces,  $\mathcal{H}_A$  and  $\mathcal{H}_B$  respectively, and where  $\{p_a\}$  form a probability distribution. It can be shown that  $k \leq (\dim(\mathcal{H}_{AB}))^2$  [156]. A quantum state of the form given in Eq. 4.1, is called a separable state. The separable states form the class of free states in QRT of entanglement as it is not possible to create entangled states by LOCC from the separable states. A state is called entangled if it is not separable. Entangled states have been a fruitful resource in various quantum information theoretic protocols. The description of the separable states can be generalized over an arbitrary number

of parties.

### 4.2.3 Quantifying entanglement

Quantification of entanglement is essential for characterization of successful preparations of quantum states, both in two party and multiparty domains. A bona-fide entanglement measure (or monotone)  $E(\rho)$  for a density operator  $\rho$  should satisfy the following two properties [12].

- *Property 1 Monotonicity:* For any LOCC,  $\mathcal{E}$  one should have

$$E(\rho) \geq E(\mathcal{E}[\rho]). \quad (4.2)$$

- *Property 2 Non-negativity:*

$$E(\rho) \geq 0. \quad (4.3)$$

The equality holds iff  $\rho$  is separable.

Moreover, there are further properties [12] that one may expect to be satisfied by a good entanglement measure, such as convexity. One may also require, for any bipartite pure state the measure of entanglement should be equal to the entropy of entanglement. Entropy of entanglement of a pure bipartite state  $|\psi\rangle_{AB}$  is given by  $S(\rho_A)$ .

#### 4.2.3.1 Bipartite entanglement

The notion of entanglement is rather well-understood in the bipartite regime, especially for pure states. While several entanglement measures can be computed for bipartite pure states, the situation for mixed states is difficult, and there are only few entanglement measures which can be computed efficiently. The logarithmic negativity [157] can be obtained for arbitrary bipartite states, while the entanglement of formation [158, 159] can be computed for all two-qubit states. We now briefly mention the entanglement of formation and the logarithmic negativity.

- *Entanglement of formation :* The entanglement of formation [158] is an entanglement measure for bipartite quantum states which is defined as

$$E_f(\rho_{AB}) = \min_{\{i\}} \sum_i p_i S(\rho_A^i), \quad (4.4)$$

where the minimization carried out over all the pure state decompositions of  $\rho_{AB}$ , such that  $\rho_{AB} = \sum_i p_i |\psi_{AB}^i\rangle\langle\psi_{AB}^i|$  and  $\rho_A^i$  is the reduced density matrix of  $|\psi_{AB}^i\rangle$ . It can be shown that entanglement formation is a monotonically increasing function of concurrence which can be computed easily. Concurrence of a two qubit system is given as  $C(\rho_{AB}) = \max\{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\}$ , where  $\lambda_1, \dots, \lambda_4$  are the square roots of the eigenvalues of  $\rho_{AB}\tilde{\rho}_{AB}$  in decreasing order,  $\tilde{\rho}_{AB} = (\sigma_y \otimes \sigma_y)\rho_{AB}^*(\sigma_y \otimes \sigma_y)$ . Here the complex conjugation  $\rho_{AB}^*$  is taken in the computational basis, and  $\sigma_y$  is the Pauli spin matrix.

- *Logarithmic negativity* : The logarithmic negativity [157] of a bipartite quantum state  $\rho_{AB}$ , is defined as

$$E_N(\rho_{AB}) = \log_2[2N(\rho_{AB}) + 1]. \quad (4.5)$$

Where,  $N(\rho_{AB}) = \frac{1}{2}(\|\rho^{\mathcal{T}A}\|_1 - 1)$  is the sum of the absolute values of the negative eigenvalues of the partial transposed density matrix of the bipartite state  $\rho_{AB}$ . Here,  $\rho^{\mathcal{T}A}$  denotes the partial transposition of  $\rho_{AB}$  with respect to  $A$ . The norm,  $\|A\|_1 = \text{Tr}\sqrt{A^\dagger A}$ , denotes the trace norm of a Hermitian matrix  $A$ .

For two qubit states, logarithmic negativity is positive if and only if the state is entangled [12]. Though, the measure is however defined and computable for bipartite states, for pure or mixed, of arbitrary dimensions, but in higher dimensions, for entangled states which have a positive partial transpose [12], the measure is vanishing. Moreover, it does not reduce to the entropy of entanglement for pure states either.

### 4.2.3.2 Multipartite entanglement

However, there have been significant advances in recent times to quantify multipartite entanglement of pure quantum states in arbitrary dimensions [12]. They are broadly classified in two categories – distance-based measures [160, 161, 162] and monogamy-based ones [163]. On the other hand, quantifying entanglement for arbitrary multiparty mixed states is still an arduous task [164].

- *Generalized Geometric Measure*: A multipartite pure quantum state  $|\psi_{A_1, A_2, \dots, A_N}\rangle$  is genuinely multipartite entangled if it is not separable across any bipartition. The Generalized Geometric Measure (GGM) [161] quantifies the genuine multipartite entanglement for these  $N$ -party states based on the distance from the

set of all multiparty states that are not genuinely entangled. The GGM is given as

$$\mathcal{G}(\psi_{A_1, A_2, \dots, A_N}) = 1 - \max_{|x\rangle} |\langle x | \psi_{A_1, A_2, \dots, A_N} \rangle|^2. \quad (4.6)$$

This maximization is done over all states  $|x\rangle$  which are not genuinely entangled. An equivalent mathematical expression of Eq.(4.6), is the following

$$\mathcal{G}(|\psi_N\rangle) = 1 - \max\{\lambda_{I:L}^2 | I \cup L = \{A_1, \dots, A_N\}, I \cap L = \emptyset\}, \quad (4.7)$$

where  $\lambda_{I:L}$  is the maximal Schmidt coefficient in the bipartite split  $I : L$  of  $|\psi_N\rangle$ . The GGM of a general mixed quantum state can be defined in terms of the convex roof construction. For an arbitrary  $N$ -party mixed state,  $\rho_N$ , the GGM can be defined as

$$\mathcal{G}(\rho_N) = \min_{\{p_i, |\psi_N^i\rangle\}} \sum_i p_i \mathcal{G}(|\psi_N^i\rangle), \quad (4.8)$$

where the minimization is over all pure state decompositions of  $\rho_N$  i.e.,  $\rho_N = \sum_i p_i |\psi_N^i\rangle\langle\psi_N^i|$ . It is difficult to find the optimal decomposition in general. However, the situation is different if the mixed quantum state under consideration possesses some symmetry. We compute the GGM, for paradigmatic classes of mixed states which have different ranks and consist of an arbitrary number of parties in Ref. [162].

## 4.3 Beyond entanglement

Apart from the measures that belong to the entanglement-separability paradigm, there are several quantum correlation measures from information theoretic paradigm. The idea of these measures were mainly conceived from thermodynamic perspectives. In particular, quantum work deficit [21], which has been pioneer in this direction was formulated based on the amount of work extracted from a quantum system coupled to a heat bath. In the following section we discuss about these measures.

### 4.3.1 Quantum work deficit

If a system is classically correlated then the amount of work  $W_l$  that can be extracted locally after suitable LOCC from the marginals are the same as the amount of work  $W_t$  that can be extracted globally when it is coupled to a heat bath [21]. Interestingly,

a quantum correlated state can allow extraction of more work globally than the work that can be extracted locally. This difference of extracted work can be used to quantify the quantum correlation present in a quantum state [21]. It is worth noting that as we are interested in the system only it is required that the operations are closed i.e., attaching ancillary system is not allowed. Therefore, it is defined as the information concentrated in a bipartite quantum state shared between two distant parties, in terms of the total work extractable under closed operation (CO) and closed local operation along with classical communication (CLOCC) [149, 150]. For a bipartite quantum state  $\rho_{AB}$ , it can be shown that the work extraction or the number of pure states that can be extracted from  $\rho_{AB}$  under CO is given by

$$W_{CO} = \log d - S(\rho_{AB}), \quad (4.9)$$

and the same under CLOCC is given by

$$W_{CLOCC} = \log d - \min_{\{P_i\}} S(\rho'_{AB}), \quad (4.10)$$

where  $d$  is the dimension of the Hilbert space of  $\rho_{AB}$  and

$$\rho'_{AB} = \sum_i (\mathbb{I}_A \otimes P_i) \rho_{AB} (\mathbb{I}_A \otimes P_i). \quad (4.11)$$

Here,  $\mathbb{I}_A$  is the identity operator on the Hilbert space of  $A$  and  $\{P_i\}$  are the set of projectors over which the minimization is carried out. Hence, the work deficit is given as

$$\mathcal{WD} = W_{CO} - W_{CLOCC}. \quad (4.12)$$

The discovery of work deficit has been conceptualized using the methods of work extraction from a quantum system when the system is in contact with a thermal bath. Thus, it has introduced a novel perspective to characterize and quantify quantum correlations from thermodynamic point of view which has been far-reaching in studying quantum correlations independent of entanglement-separability paradigm. It also further strengthens the link between thermodynamics and quantum information theory.

### 4.3.2 Quantum discord

Quantum discord is a measure of quantum correlations of bipartite quantum states that is independent of the entanglement-separability paradigm [22, 138, 139]. It

can be conceptualized from several perspectives. An approach that is intuitively satisfying, is to define it as the difference between the total correlation and the classical correlation for a bipartite quantum state  $\rho_{AB}$ . The total correlation is defined as the quantum mutual information of  $\rho_{AB}$ , which is given by

$$\mathcal{I}(\rho_{AB}) = S(\rho_A) + S(\rho_B) - S(\rho_{AB}), \quad (4.13)$$

where  $\rho_A$  and  $\rho_B$  are the local density matrices of  $\rho_{AB}$ . The mutual information  $\mathcal{I}(\rho_{AB})$  can also be expressed in terms of the usual quantum relative entropy as

$$\mathcal{I}(\rho_{AB}) = \min_{\{\sigma_A, \sigma_B\}} S(\rho_{AB} || \sigma_A \otimes \sigma_B). \quad (4.14)$$

This follows from  $\min_{\{\sigma_A, \sigma_B\}} S(\rho_{AB} || \sigma_A \otimes \sigma_B) = \min_{\{\sigma_A, \sigma_B\}} \{-S(\rho_{AB}) - \text{Tr}(\rho_A \log \sigma_A) - \text{Tr}(\rho_B \log \sigma_B)\}$ , and the non-negativity of relative von Neumann entropy between two density matrices. Therefore, the quantum mutual information is the minimum usual relative entropy distance of the state  $\rho_{AB}$  from the set of all completely uncorrelated states,  $\sigma_A \otimes \sigma_B$ , whence we obtain a ground for interpreting the quantum mutual information as the total correlation in the state. The classical correlation is given in terms of the measured conditional entropy, and is defined as [138, 139]

$$\mathcal{J}(\rho_{AB}) = S(\rho_A) - S(\rho_{A|B}), \quad (4.15)$$

where

$$S(\rho_{A|B}) = \min_{\{P_i\}} \sum_i p_i S(\rho_{A|i}) \quad (4.16)$$

is the conditional entropy of  $\rho_{AB}$ , conditioned on measurements at  $B$  with rank-one projection-valued measurements  $\{P_i\}$ . Here,  $\rho_{A|i} = \frac{1}{p_i} \text{Tr}_B[(\mathbb{I}_A \otimes P_i)\rho(\mathbb{I}_A \otimes P_i)]$  is the conditional state which we get with probability  $p_i = \text{Tr}_{AB}[(\mathbb{I}_A \otimes P_i)\rho(\mathbb{I}_A \otimes P_i)]$ , where  $\mathbb{I}_A$  is the identity operator on the Hilbert space of  $A$ . It is worth mentioning that the minimization need not be done over projection-valued measurements in general, as it can be performed over more general measurements called POVMs [138]. However, since this is computationally difficult, often for convenience in the definition of quantum discord, work deficit etc. the minimization is restricted to projective measurements. In this thesis we will also be restricted to projective measurements to maximize the classical correlations.  $\mathcal{J}(\rho_{AB})$  can also be defined in terms of the mutual information as

$$\mathcal{J}(\rho_{AB}) = \max_{\{P_i\}} \mathcal{I}(\rho'_{AB}), \quad (4.17)$$

where

$$\rho'_{AB} = \sum_i (\mathbb{I}_A \otimes P_i) \rho_{AB} (\mathbb{I}_A \otimes P_i). \quad (4.18)$$

The classical correlation can therefore be seen as the minimum relative entropy distance of the state  $\rho'_{AB}$  from all uncorrelated states, maximized over all rank-one projective measurements on  $B$ , and is given by

$$\mathcal{J}(\rho_{AB}) = \max_{\{P_i\}} \min_{\{\sigma_A, \sigma_B\}} S(\rho'_{AB} || \sigma_A \otimes \sigma_B). \quad (4.19)$$

The maximization in Eq. (4.19) or in Eq. (4.15) ensure that  $\mathcal{J}(\rho_{AB})$  quantifies the maximal content of classical correlation present in the bipartite state  $\rho_{AB}$ . Hence, if we subtract  $\mathcal{J}(\rho_{AB})$  from the total correlation, the remaining correlation is “purely” quantum, and is defined as [138, 139]

$$\mathcal{D}(\rho_{AB}) = \mathcal{I}(\rho_{AB}) - \mathcal{J}(\rho_{AB}). \quad (4.20)$$

Quantum discord plays a significant role in quantum thermodynamics. Zurek has defined quantum thermal discord taking the entropic cost of the measurement which is crucial when one considers thermodynamic scenario [165]. In Ref. [165], a thermodynamic interpretation of quantum discord has also been given by pointing out that quantum discord can be thought of as the difference between the work extracted by the quantum and classical demons respectively. Later it has been shown by Aharon and Daniel [24] that discord can determine the difference between efficiencies in Szilard’s engine under different restrictions. These results have further cemented the link between quantum correlations and thermodynamics. Moreover, quantum discord has been extensively used to study co-operative phenomena in quantum many-body physics [22, 166, 167, 168, 169]. We refer the reader to the nice review [22] for more details.

## 4.4 Chapter summary

In this chapter, we have studied bipartite and multipartite measures of quantum correlations both entanglement and measure that are beyond entanglement. We have also studied the QRT of entanglement in brief. In the next chapter, we will see that quantum discords defined using generalized entropies are advantageous to detect criticality in transverse field quantum Ising model.

# Generalized quantum correlation and quantum phase transition

## 5.1 Introduction

In classical as well as quantum information theory, one of the most important pillars is the framework of entropy [170], which quantifies the ignorance or lack of information about a relevant physical system. Moreover, it helps to understand information theory from a thermodynamic perspective. Almost all the quantum correlation measures incorporate entropic functions in various forms. And, most of the quantum correlation measures are defined by using the von Neumann entropy. The operational significance of von Neumann entropy has been widely recognized in numerous scenarios in quantum information theory. Nonetheless, there are classes of generalized entropies like the Rényi [171] and Tsallis [172] entropies, which are also operationally significant in important physical scenarios. Both the Rényi and Tsallis entropies reduce to the von Neumann entropy when the entropic parameter  $\alpha \rightarrow 1$ . For  $\alpha \in (0, 1)$ , the relative Rényi entropy appears in the quantum Chernoff bound which determines the minimal probability of error in discriminating two different quantum states in the setting of asymptotically many copies [173]. In Ref. [174], it was shown that the relative Rényi entropy is relevant in binary quantum state discrimination, for the same range of  $\alpha$ . The concept of Rényi entropy has also been found to be useful in the context of holographic theory [175, 176, 177]. It has also been found useful in dealing with several condensed matter systems [178, 179, 180, 181, 182, 183]. The significance of the Tsallis entropy in quantum information theory has been established in the context of quantifying entanglement [184], local realism [185], and

entropic uncertainty relations [186] (see also [187, 188]). Both the Rényi and Tsallis entropies have important applications in classical as well as quantum statistical mechanics and thermodynamics [189].

While there are important interpretational and operational breakthroughs that have been obtained by using the concept of quantum discord, there are also several intriguing unanswered questions and thriving controversies [22, 190]. It is therefore interesting and important to look back upon the conceptual foundations of quantum discord and inquire whether certain changes, subtle or substantial, in those concepts lead us to a better understanding of the controversies and the unanswered questions. Towards this aim, in this chapter, we introduce measures of the total, classical, and quantum correlations of a bipartite quantum state in terms of the entire class of relative Rényi and Tsallis entropy distances. We first show that the measures satisfy all the required properties of bipartite correlations. We then evaluate the quantum correlation measure for several paradigmatic classes of states. As an application, we find that the quantum correlation measures, via relative Rényi and Tsallis entropies, can indicate quantum phase transitions and give better finite-size scaling exponents than the other known order parameters. Importantly, we show that the conceptualization of the measures in terms of Rényi and Tsallis entropies solves an incommodious feature regarding the behavior of nearest-neighbor quantum discord in a second order phase transition.

There are two distinct ways in which the relative Rényi and Tsallis entropies are defined, and are usually referred to as the “traditional” [191, 192] and “sandwiched” [193, 194] varieties. The sandwiched varieties incorporate the noncommutative nature of density matrices in an elegant way, and it is therefore natural to expect that it will play an important role in fundamentals and applications. Indeed, the sandwiched relative Rényi entropy has been used to show that the strong converse theorem for the classical capacity of a quantum channel holds for some specific channels [193]. Moreover, an operational interpretation of the sandwiched relative Rényi entropy in the strong converse problem of quantum hypothesis testing is noted for  $\alpha > 1$  [195]. On the other hand, the sandwiched relative Tsallis entropy has recently been shown to be a better witness of entanglement [196] than the traditional one [184]. The relative min- and max-entropies [197, 198], which can be obtained from the sandwiched relative Rényi entropy for specific choices of  $\alpha$ , play significant roles in providing bounds on errors of one-shot entanglement cost [199], on the one-shot classical capacity of certain quantum channels [200], and in several scenarios in non-asymptotic quantum information theory [201]. In Ref. [202], connection

of max- relative entropy with frustration in quantum many body systems has been established.

## 5.2 Relative Rényi and Tsallis entropies

To define quantum discord in terms generalized entropies, we first introduce the generalized entropies and their relative versions in this section. We will also discuss the useful properties of these quantities which will be used to define the quantum correlations. The Rényi [171, 203, 204] and Tsallis [172, 205] entropies of a density operator  $\rho$  are given respectively by

$$S_\alpha^R(\rho) = \frac{1}{1-\alpha} \log \text{Tr}[\rho^\alpha], \quad (5.1)$$

$$S_\alpha^T(\rho) = \frac{\text{Tr}[\rho^\alpha] - 1}{1-\alpha}. \quad (5.2)$$

Here, the parameter  $\alpha \in (0, 1) \cup (1, \infty)$ , unless mentioned otherwise. All logarithms in this chapter are with base 2. Both the entropies reduce to the von Neumann entropy [206],  $S(\rho) = -\text{Tr}(\rho \log \rho)$ , when  $\alpha \rightarrow 1$ . The Tsallis entropy for  $\alpha = 2$  is called the linear entropy,  $S_L(\rho)$ , given by

$$S_L(\rho) = 1 - \text{Tr}[\rho^2]. \quad (5.3)$$

The traditional quantum relative Rényi entropy between two density operators  $\rho$  and  $\sigma$  is defined as

$$S_\alpha^R(\rho||\sigma) = \frac{\log \text{Tr}[(\rho^\alpha \sigma^{1-\alpha})]}{\alpha - 1}. \quad (5.4)$$

Note that all the quantum relative entropies, traditional or sandwiched, discussed in this chapter, are defined to be  $+\infty$  if the kernel of  $\sigma$  has non-trivial intersection with the support of  $\rho$ , and is finite otherwise.  $S_\alpha^R(\rho||\sigma)$  reduces to the usual quantum relative entropy [207, 208],  $S(\rho||\sigma)$ , when  $\alpha \rightarrow 1$ , where

$$S(\rho||\sigma) = -S(\rho) - \text{Tr}(\rho \log \sigma). \quad (5.5)$$

Recently, a generalized version of the quantum relative Rényi entropy (called “sandwiched” relative Rényi entropy) has been introduced, by considering the non commutative nature of density operators [193, 194]. It is defined as

$$\tilde{S}_\alpha^R(\rho||\sigma) = \frac{1}{\alpha - 1} \log \text{Tr} \left[ \left( \sigma^{\frac{1-\alpha}{2\alpha}} \rho \sigma^{\frac{1-\alpha}{2\alpha}} \right)^\alpha \right]. \quad (5.6)$$

Note that  $\tilde{S}_\alpha^R(\rho||\sigma)$  also reduces to  $S(\rho||\sigma)$  when  $\alpha \rightarrow 1$ . In Ref. [100, 193, 194, 209, 210] several interesting properties of the sandwiched Rényi entropy have been established. Here, we mention some of them (for two density operators  $\rho$  and  $\sigma$ ) which we will use later in this chapter.

1.  $\tilde{S}_\alpha^R(\rho||\sigma) \geq 0$ .
2.  $\tilde{S}_\alpha^R(\rho||\sigma) = 0$  if and only if  $\rho = \sigma$ .
3. For  $\alpha \in [\frac{1}{2}, 1) \cup (1, \infty)$  and for any completely positive trace-preserving map (CPTPM)  $\mathcal{E}$ , we have the data processing inequality,  $\tilde{S}_\alpha^R(\rho||\sigma) \geq \tilde{S}_\alpha^R(\mathcal{E}(\rho)||\mathcal{E}(\sigma))$  [210]. The data processing inequality holds as  $\exp[(\alpha - 1)\tilde{S}_\alpha^R(\rho||\sigma)]$  is jointly convex for  $\alpha \in (1, \infty)$  and jointly concave for  $\alpha \in [\frac{1}{2}, 1)$ . There are numerical evidences that data processing inequality does not hold for  $\alpha < \frac{1}{2}$ .
4.  $\tilde{S}_\alpha^R(\rho||\sigma)$  is invariant under all unitaries  $U$ , i.e.,  $\tilde{S}_\alpha^R(U\rho U^\dagger||U\sigma U^\dagger) = \tilde{S}_\alpha^R(\rho||\sigma)$ .

The traditional quantum relative Tsallis entropy between two density operators  $\rho$  and  $\sigma$  is defined as

$$S_\alpha^T(\rho||\sigma) = \frac{\text{Tr}(\rho^\alpha \sigma^{1-\alpha}) - 1}{\alpha - 1}. \quad (5.7)$$

The sandwiched relative Tsallis entropy between two density operators  $\rho$  and  $\sigma$  is given by [196]

$$\tilde{S}_\alpha^T(\rho||\sigma) = \frac{\text{Tr} \left[ \left( \sigma^{\frac{1-\alpha}{2\alpha}} \rho \sigma^{\frac{1-\alpha}{2\alpha}} \right)^\alpha \right] - 1}{\alpha - 1}. \quad (5.8)$$

Both  $S_\alpha^T(\rho||\sigma)$  and  $\tilde{S}_\alpha^T(\rho||\sigma)$  also reduce to  $S(\rho||\sigma)$  when  $\alpha \rightarrow 1$ . It can be easily verified that the properties (1-4), satisfied by  $\tilde{S}_\alpha^R(\rho||\sigma)$  are also satisfied by  $\tilde{S}_\alpha^T(\rho||\sigma)$ . In this chapter, we will predominantly use the sandwiched version of both the relative entropies. Hereafter, by relative entropy, we will mean the sandwiched form of the relative entropies, unless mentioned otherwise. Some of the important special cases of the Rényi and Tsallis relative entropies are given below.

**a. Relative linear entropy :** At  $\alpha = 2$ ,  $\tilde{S}_\alpha^T(\rho||\sigma)$  gives the relative linear entropy,

$$S_L(\rho||\sigma) = \tilde{S}_2^T(\rho||\sigma). \quad (5.9)$$

The relative linear entropy has also been defined in the literature by using the traditional version of the relative entropy at  $\alpha = 2$ . However, in this chapter, we will use the relative linear entropy defined only through the sandwiched relative entropy (at  $\alpha = 2$ ).

**b. Relative collision entropy :** At  $\alpha = 2$ ,  $\tilde{S}_\alpha^R(\rho||\sigma)$  has been called the relative collision entropy [197],

$$S_C(\rho||\sigma) = \tilde{S}_2^R(\rho||\sigma). \quad (5.10)$$

**c. Relative min- and max-entropies :** In Ref. [198], it is pointed out that at  $\alpha = \frac{1}{2}$ ,  $\tilde{S}_\alpha^R(\rho||\sigma)$  gives relative min-entropy [211],

$$S_{min}(\rho||\sigma) = \tilde{S}_{\frac{1}{2}}^R(\rho||\sigma). \quad (5.11)$$

Note that

$$S_{min}(\rho||\sigma) = -2 \log F(\rho, \sigma), \quad (5.12)$$

where  $F(\rho, \sigma) = \|\sqrt{\rho}\sqrt{\sigma}\|_1 = \text{Tr}|\sqrt{\rho}\sqrt{\sigma}|$  is the fidelity between the states  $\rho$  and  $\sigma$ . It is shown in Ref. [194], that the relative max-entropy [198] is nothing but relative Rényi entropy, when  $\alpha \rightarrow \infty$  i.e.

$$S_{max}(\rho||\sigma) = \tilde{S}_{\alpha \rightarrow \infty}^R(\rho||\sigma), \quad (5.13)$$

where

$$S_{max}(\rho||\sigma) = \inf(\lambda : \rho \leq 2^\lambda \sigma). \quad (5.14)$$

## 5.3 Total, classical, and quantum correlations as relative entropies

In this section, we define the total, classical, and quantum correlation in terms of the sandwiched relative Rényi and Tsallis entropies. We discuss the properties of these measures and evaluate them for several important families of bipartite quantum states. In the final subsection, we also compare the results with those obtained with traditional relative entropies.

### 5.3.1 Generalized mutual information as total correlation

We define the generalized mutual information of  $\rho_{AB}$  as

$$\mathcal{I}_\alpha^\Gamma(\rho_{AB}) = \min_{\{\sigma_A, \sigma_B\}} \tilde{S}_\alpha^\Gamma(\rho_{AB}||\sigma_A \otimes \sigma_B). \quad (5.15)$$

Here, the minimum is taken over all density matrices,  $\sigma_A$  and  $\sigma_B$ . The relative entropy, although not a metric on the operator space, is a measure of the distance between two quantum states.  $\tilde{S}_\alpha^\Gamma(\rho_{AB}||\sigma_A \otimes \sigma_B)$  is a distance between the quantum state  $\rho_{AB}$  and a completely uncorrelated state  $\sigma_A \otimes \sigma_B$ . Here, and hereafter, the superscript  $\Gamma$  is either  $R$  or  $T$ , depending on whether it is the Rényi or Tsallis variety that is considered. The corresponding minimum distance can be interpreted as the total correlation present in the system. The generalized mutual information  $\mathcal{I}_\alpha^\Gamma(\rho_{AB})$  becomes equal to the usual quantum mutual information  $\mathcal{I}(\rho_{AB})$  when  $\alpha \rightarrow 1$ :

$$\begin{aligned} \lim_{\alpha \rightarrow 1} \mathcal{I}_\alpha^\Gamma(\rho_{AB}) &= \lim_{\alpha \rightarrow 1} \min_{\{\sigma_A, \sigma_B\}} \tilde{S}_\alpha^\Gamma(\rho_{AB}||\sigma_A \otimes \sigma_B). \\ &= \min_{\{\sigma_A, \sigma_B\}} S(\rho_{AB}||\sigma_A \otimes \sigma_B) \\ &\equiv \mathcal{I}(\rho_{AB}). \end{aligned} \tag{5.16}$$

### 5.3.2 Classical and quantum correlation

The Rényi or Tsallis version of the classical correlation, denoted by  $\mathcal{J}_\alpha^\Gamma(\rho_{AB})$ , is defined as

$$\mathcal{J}_\alpha^\Gamma(\rho_{AB}) = \max_{\{P_i\}} \min_{\{\sigma_A, \sigma_B\}} \tilde{S}_\alpha^\Gamma(\rho'_{AB}||\sigma_A \otimes \sigma_B), \tag{5.17}$$

where  $\rho'_{AB}$  is obtained by performing rank-1 projective measurements as in the definition of original classical correlation (in Eq. (4.18)).

Therefore, quantum correlation using generalized entropies is defined as

$$\mathcal{D}_\alpha^\Gamma(\rho_{AB}) = \mathcal{I}_\alpha^\Gamma(\rho_{AB}) - \mathcal{J}_\alpha^\Gamma(\rho_{AB}), \tag{5.18}$$

with  $\alpha \in [\frac{1}{2}, 1) \cup (1, \infty)$ . By using the data processing inequality, which holds in this range of  $\alpha$ , one can prove the non-negativity of the quantum correlation [210]. We now look into the properties of  $\mathcal{D}_\alpha^\Gamma(\rho_{AB})$ , which provide independent support for identifying the quantities as correlation measures.

**Property 1**  $\mathcal{I}_\alpha^\Gamma, \mathcal{J}_\alpha^\Gamma \geq 0$  since  $\tilde{S}_\alpha^\Gamma(\rho||\sigma) \geq 0$ .

**Property 2**  $\mathcal{I}_\alpha^\Gamma, \mathcal{J}_\alpha^\Gamma$  are vanishing, and therefore,  $\mathcal{D}_\alpha^\Gamma = 0$ , for any product state,  $\rho_{AB} = \rho_A \otimes \rho_B$ , as  $\tilde{S}_\alpha^R(\rho||\rho) = 0$ . The proof for the vanishing of total correlations follows by noting that the product state in the argument itself is the state which gives the optimal relative entropy distance. A similar argument, but for the measured state, holds for the classical correlation.

Moreover,  $\mathcal{D}_\alpha^\Gamma = 0$  for any quantum-classical state, i.e. any state of the form

$\sum_i p_i \rho_i^A \otimes (|i\rangle\langle i|)^B$ , where  $\{p_i\}$  forms a probability distribution,  $\{|i\rangle\}$  forms an orthonormal basis, and  $\rho_i$  are density matrices, when the measurement is performed on the  $B$  part.

**Property 3**  $\mathcal{I}_\alpha^I, \mathcal{J}_\alpha^I$  remain invariant under local unitaries, which follow from the fact that  $\tilde{S}_\alpha^R(\rho||\sigma)$  is invariant under all unitaries  $U$ . Hence,  $\mathcal{D}_\alpha^I$  is also invariant under local unitaries.

**Property 4**  $\mathcal{I}_\alpha^I, \mathcal{J}_\alpha^I$  are non increasing under local operations, which follow from the data processing inequality,  $\tilde{S}_\alpha^R(\rho||\sigma) \geq \tilde{S}_\alpha^R(\mathcal{E}(\rho)||\mathcal{E}(\sigma))$ , for any CPTPM  $\mathcal{E}$ .

**Property 5**  $\mathcal{D}_\alpha^I$  is non-negative, as  $\mathcal{J}_\alpha^I$  is upper bounded by  $\mathcal{I}_\alpha^I$ . The latter statement is due to the fact that  $\mathcal{J}_\alpha^I$  is obtained by performing a local measurement on  $\rho_{AB}$ , and we know from the data processing inequality that  $\tilde{S}_\alpha^I$  is monotone under CPTPM.

As the property 4 and 5 which hold due to the data processing inequality, are crucial for quantum and classical correlation, we define the same in the range  $\alpha \in [\frac{1}{2}, 1) \cup (1, \infty)$ . The classical correlation measure that we have defined here, satisfies all the plausible properties for classical correlation proposed in Ref. [138], except the one which states that for pure states, the classical correlation reduces to the von Neumann entropy of the subsystems. We wish to mention that this property is natural for the measure which involves the von Neumann entropy, and is not expected to be followed by the measures with generalized entropies. This is because the definition of classical correlation in terms of the relative entropy reduces naturally to the one in terms of the conditional entropy in the case of the von Neumann entropy.

We use the convention that each of the definitions of  $\mathcal{I}_\alpha^I, \mathcal{J}_\alpha^I$  and  $\mathcal{D}_\alpha^I$  also incorporates a division by  $\log 2$  bits, whence all the definitions can be considered to be dimensionless.

We note here that there has been previous attempts to define quantum discord by using Tsallis entropies [212, 213, 214]. These definitions however do not always guarantee positivity of the quantum discord, so defined. Also, the corresponding total and classical correlations are not necessarily monotonic under local operations. Ref. [215] defines a quantum correlation by considering the difference between the Tsallis entropies of the post-measured and pre-measured states. In Ref. [216], a Gaussian quantum correlation is defined by using the Rényi entropy for  $\alpha = 2$ . Generalized quantum discord based on the Rényi entropy has been defined of late in Ref. [217] following different approach.

### 5.3.3 Special cases

#### 5.3.3.1 Linear quantum discord

The relative linear entropy can be used to define the “linear quantum discord”, given by

$$\mathcal{D}_L(\rho_{AB}) = \mathcal{I}_2^T(\rho_{AB}) - \mathcal{J}_2^T(\rho_{AB}), \quad (5.19)$$

where  $\mathcal{I}_2^T(\rho_{AB})$  and  $\mathcal{J}_2^T(\rho_{AB})$  are defined by using the relative linear entropy, given in Eq. (5.9).

#### 5.3.3.2 Min- and max-quantum discords

We also define the “min- and max-quantum discords” by considering relative min- and max-entropies as

$$\mathcal{D}_{min}(\rho_{AB}) = \mathcal{I}_{\frac{1}{2}}^R(\rho_{AB}) - \mathcal{J}_{\frac{1}{2}}^R(\rho_{AB}), \quad (5.20)$$

and

$$\mathcal{D}_{max}(\rho_{AB}) = \mathcal{I}_{\alpha \rightarrow \infty}^R(\rho_{AB}) - \mathcal{J}_{\alpha \rightarrow \infty}^R(\rho_{AB}). \quad (5.21)$$

### 5.3.4 Generalized discord of pure states

Any bipartite pure state of two qubits can be written, using Schmidt decomposition, as

$$|\psi_{AB}\rangle = \sum_{i=0}^1 \sqrt{\lambda_i} |i_A i_B\rangle, \quad (5.22)$$

where  $\lambda_i$  are non-negative real numbers satisfying  $\sum_i \lambda_i = 1$ . Since a bipartite pure state is symmetric, it is expected that the state  $\sigma_A \otimes \sigma_B$ , which minimizes the relative entropy of  $|\psi_{AB}\rangle$  with uncorrelated states, is also symmetric. Numerical studies support this view. This fact is not only true for pure bipartite states, but it holds for all symmetric bipartite states that are considered in this chapter. Moreover, numerical results indicate that for arbitrary  $|\psi_{AB}\rangle$ , the state  $\sigma^A \otimes \sigma^B$  which gives the minimum, is diagonal in the Schmidt basis of  $|\psi_{AB}\rangle$ . To numerically evaluate the minimum relative entropy distance of a bipartite quantum state  $\rho_{AB}$  from product states, we begin by randomly generating bipartite product states  $\sigma_A \otimes \sigma_B$ . Then we calculate the relative entropies between  $\rho_{AB}$  and all such  $\sigma_A \otimes \sigma_B$ . The minimum of these relative entropies is considered to be the minimum relative entropy distance. We repeat the procedure for a larger set of randomly chosen product states. We

terminate the process when the minimum does not change within the required precision <sup>1</sup>. Note that the numerical study is performed without the assumptions that the product state at which the minimum is attained is symmetric and that it is diagonal in the Schmidt basis. We have followed the same procedure throughout the chapter to numerically evaluate the different correlations. Therefore, the minimum  $\sigma_A$  or  $\sigma_B$  is given by

$$\sigma_A = \sigma_B = \sigma \equiv \sum_{i=0}^1 a_i |i\rangle\langle i|, \quad (5.23)$$

where  $a_i$  are non-negative real numbers satisfying  $\sum_i a_i = 1$ . With these assumptions, the total correlation of  $|\psi_{AB}\rangle$  is given by

$$\mathcal{I}_\alpha^R(|\psi_{AB}\rangle) = \min_{\{a\}} \frac{1}{\alpha - 1} \log \left[ \lambda a^{\frac{2(1-\alpha)}{\alpha}} + (1-\lambda)(1-a)^{\frac{2(1-\alpha)}{\alpha}} \right]^\alpha, \quad (5.24)$$

where  $a_0 = a$ ,  $a_1 = 1 - a$ ,  $\lambda_0 = \lambda$ ,  $\lambda_1 = 1 - \lambda$ . The value of  $a$  is obtained from the condition

$$\frac{1}{a} = \left( \frac{\lambda}{1-\lambda} \right)^{\frac{\alpha}{2-3\alpha}} + 1, \quad (5.25)$$

for  $\alpha \in (2/3, 1) \cup (1, \infty)$ . For  $\frac{1}{2} \leq \alpha \leq \frac{2}{3}$ , the minimization in Eq. (5.24) yields

$$\mathcal{I}_\alpha^R(|\psi_{AB}\rangle) = \frac{\alpha}{\alpha - 1} \log [\max\{\lambda, 1 - \lambda\}]. \quad (5.26)$$

For pure states, numerical searches indicate that the classical correlation is independent of the measurement basis. We consider measurement performed in the Schmidt basis for calculating the classical correlation of the original state. Just like the total correlation in the original state, the  $\sigma_A \otimes \sigma_B$ , which minimizes the relative entropy of the post-measurement state with uncorrelated states, is symmetric, since we perform the projective measurement in the Schmidt basis. Moreover, from numerical results, we find that  $\sigma_A \otimes \sigma_B$  is again diagonal in the Schmidt basis of  $|\psi_{AB}\rangle$ . The Rényi classical correlation of  $|\psi_{AB}\rangle$  is therefore given by

$$\mathcal{J}_\alpha^R(|\psi_{AB}\rangle) = \min_{\{a\}} \frac{1}{\alpha - 1} \log \left[ \lambda^\alpha a^{2(1-\alpha)} + (1-\lambda)^\alpha (1-a)^{2(1-\alpha)} \right]. \quad (5.27)$$

---

<sup>1</sup>We would like to mention that we have generated  $10^6 - 10^7$  product states in the two qubit Hilbert space to check all the numerical results presented in this chapter. However, we have found that the measure converges satisfactorily enough even within  $10^5$  number of states.

The value of  $a$  is obtained from the condition

$$\frac{1}{a} = \left( \frac{\lambda}{1-\lambda} \right)^{\frac{\alpha}{1-2\alpha}} + 1, \quad (5.28)$$

for  $\alpha \in (1/2, 1) \cup (1, \infty)$ .

The linear quantum discord for  $|\psi_{AB}\rangle$  is given by

$$\mathcal{D}_L(|\psi_{AB}\rangle) = (\sqrt{\lambda} + \sqrt{1-\lambda})^4 - (\sqrt{\lambda} + \sqrt{1-\lambda})^2. \quad (5.29)$$

We find that the min-quantum discord is vanishing for every two-qubit pure state. We believe that this is a peculiarity of some elements of the class of information-theoretic quantum correlation measures that are defined according to the premise that subtracting classical correlations from total correlations will produce quantum correlations. This may perhaps be paralleled with the fact that although it was perhaps considered desirable that all entanglement measures should possess the property that they should vanish for separable states and only for separable states, the discovery of bound entangled states [218, 219] led us to the fact that distillable entanglement [220, 221, 222] can vanish for certain entangled states as well. It should be noted that in contradistinction to distillable entanglement, the min-quantum discord can be non-zero for certain separable states, indicating that at least in this sense, the space of information-theoretic quantum correlations is richer than the space of entanglement measures.

The max-quantum discord for  $|\psi_{AB}\rangle$  is given by

$$\mathcal{D}_{max}(|\psi_{AB}\rangle) = \log \left[ \frac{(\sqrt[3]{\lambda} + \sqrt[3]{1-\lambda})^3}{(\sqrt{\lambda} + \sqrt{1-\lambda})^2} \right]. \quad (5.30)$$

In Fig. 5.1, we plot the Rényi quantum correlation of  $|\psi_{AB}\rangle$  for various values of  $\alpha$ . We have also performed the entire calculations for the Tsallis discord and find that its behavior is qualitatively similar to the Rényi discord. In Fig. 5.2, we have exhibited the Tsallis discord for bipartite pure states, which clearly indicate the similarity between the two discords. In the rest of the chapter, we will only plot the Rényi discord.

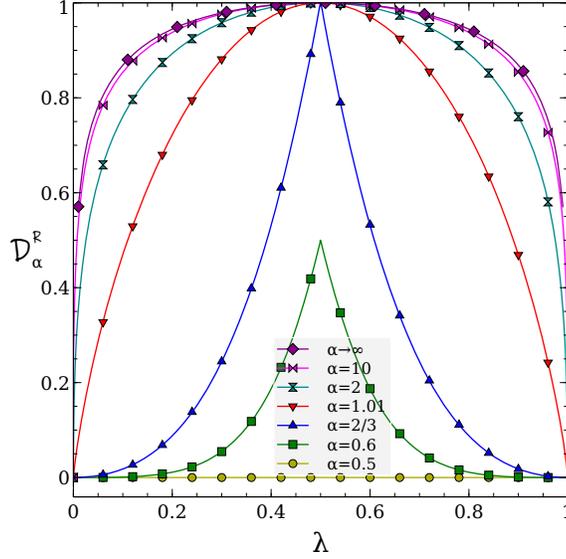


Figure 5.1: Rényi quantum correlation,  $\mathcal{D}_\alpha^R$ , with respect to  $\lambda$ , of  $|\psi_{AB}\rangle = \sqrt{\lambda}|00\rangle + \sqrt{(1-\lambda)}|11\rangle$ , for different  $\alpha$ . Both axes are dimensionless.

### 5.3.5 Generalized discord of mixed states: Some examples

(i) **Werner states:** Consider the Werner state, given by

$$\rho_W = p|\psi^-\rangle\langle\psi^-| + (1-p)\frac{I}{4},$$

where  $|\psi^-\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$ ,  $I$  denotes the identity operator on the two-qubit Hilbert space, and  $0 \leq p \leq 1$ . Suppose the  $\sigma_A^{min}$  and  $\sigma_B^{min}$  are the optimal  $\sigma_A$  and  $\sigma_B$  which minimizes the relative Rényi entropy of  $\rho_W$  with uncorrelated states. Using the fact that the Werner state is symmetric and local unitarily invariant, we choose

$$\sigma_A^{min} = \sigma_B^{min} = \sigma \equiv a_0|0\rangle\langle 0| + a_1|1\rangle\langle 1|, \quad (5.31)$$

where  $a_i$  are non-negative real numbers satisfying  $\sum_i a_i = 1$ . Here we have assumed that  $\sigma_A \otimes \sigma_B$ , which minimizes the relative entropy of  $\rho_W$  with uncorrelated states, is symmetric. Detail numerical study support our assumption, as mentioned in Sec. 5.3.4. It is now possible to perform the minimization for  $\alpha \in [\frac{2}{3}, 1) \cup (1, \infty)$ . In this range, the relative Rényi entropy distance corresponding to the total correlations is minimum for  $a_0 = a_1 = \frac{1}{2}$ . Therefore, the Rényi total correlation of the Werner state

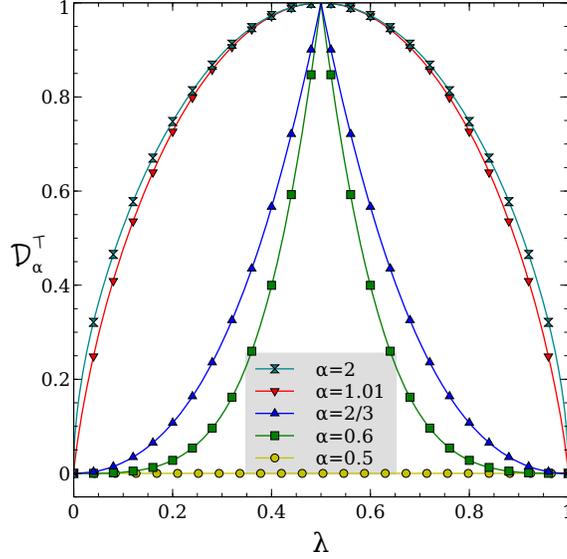


Figure 5.2: Tsallis quantum correlation,  $\mathcal{D}_\alpha^T$ , with respect to  $\lambda$ , of  $|\psi_{AB}\rangle = \sqrt{\lambda}|00\rangle + \sqrt{(1-\lambda)}|11\rangle$ , for different  $\alpha$ . Both axes are dimensionless. The values of the Tsallis quantum correlation are normalized, whenever possible, so that the maximal quantum correlations are of unit value.

for  $\alpha \geq \frac{2}{3}$  ( $\alpha \neq 1$ ) is given by

$$\mathcal{I}_\alpha^R(\rho_W) = 2 + \frac{1}{\alpha - 1} \log \frac{1}{4^\alpha} [(1 + 3p)^\alpha + 3(1 - p)^\alpha]. \quad (5.32)$$

Just like for the case of pure bipartite states, the Rényi classical correlation is again independent of measurement basis, as is expected from the property of rotational invariance of the Werner state.

Numerical observations also suggest that for  $\alpha \geq \frac{1}{2}$  ( $\alpha \neq 1$ ) and for any  $p$ , the relative Rényi entropy is minimum at  $\sigma_A \otimes \sigma_B = \frac{I}{4}$  for the post-measurement state corresponding to the Werner state. So the Rényi classical correlation, in this range of  $\alpha$ , is given by

$$\mathcal{J}_\alpha^R(\rho_W) = 2 + \frac{1}{\alpha - 1} \log \frac{1}{4^\alpha} [2(1 + p)^\alpha + 2(1 - p)^\alpha]. \quad (5.33)$$

Hence, the Rényi quantum correlation of the Werner state for  $\alpha \geq \frac{2}{3}$  ( $\alpha \neq 1$ ) is given by

$$\mathcal{D}_\alpha^R(\rho_W) = \frac{1}{\alpha - 1} \log \left[ \frac{(1 + 3p)^\alpha + 3(1 - p)^\alpha}{2(1 + p)^\alpha + 2(1 - p)^\alpha} \right]. \quad (5.34)$$

For  $\frac{1}{2} \leq \alpha < \frac{2}{3}$ , we find the Rényi quantum correlation for the Werner states by

numerical evaluation. In Fig. 5.3, we exhibit the Rényi quantum correlation for the Werner states for different values of  $\alpha$ .

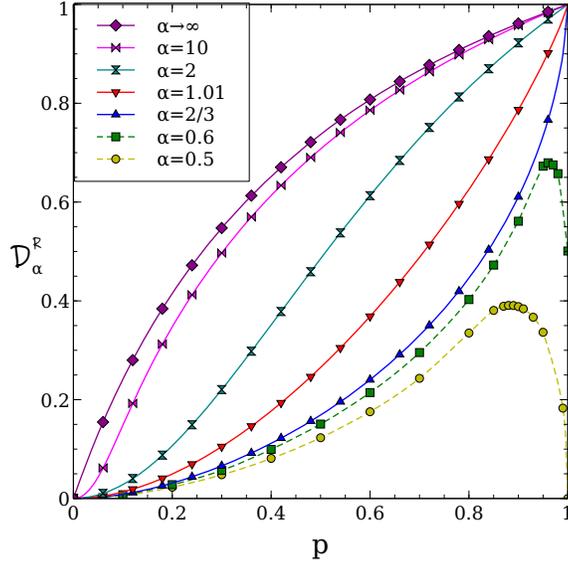


Figure 5.3: Rényi quantum correlation,  $\mathcal{D}_\alpha^R$ , with respect to  $p$ , of the Werner state,  $\rho_W = p|\psi^-\rangle\langle\psi^-| + (1-p)\frac{1}{4}I$ , for different  $\alpha$ . Both axes are dimensionless.

The Rényi quantum correlation is maximum for the Werner state at  $p = 1$  for  $\alpha \geq \frac{2}{3}$ . The singlet state, and states that are local unitarily connected with it, is therefore maximally Rényi quantum correlated in that range of  $\alpha$ , among the Werner states. However, for  $\frac{1}{2} \leq \alpha < \frac{2}{3}$ , the Bell states are not the maximally Rényi quantum correlated states. In this range of  $\alpha$ , we get maximal quantum correlation among the Werner states, for a value of  $p$  that is different from unity. For example, for  $\alpha = 0.6$ , we find that the state,  $\rho_W$ , with mixing parameter  $p \approx 0.96$  has the maximal quantum correlation among all Werner states. For  $\alpha = 1/2$ , the same is at  $p \approx 0.88$ . For  $\alpha = \frac{1}{2}$ , i.e., for min-entropy, the singlet has zero quantum correlation. Indeed, all pure states have vanishing min-quantum discord. We will visit this issue again in Sec. 5.3.6.

The linear quantum discord for the Werner state is

$$\mathcal{D}_L(\rho_W) = \frac{1}{4} [(1+3p)^2 + (1-p)^2 - 2(1+p)^2]. \quad (5.35)$$

The max-quantum discord can also be calculated similarly for the Werner state and is given by

$$\mathcal{D}_{max}(\rho_W) = \log \left[ \frac{(1+3p)}{(1+p)} \right]. \quad (5.36)$$

We have numerically evaluated the min-quantum discord for the Werner state (see Fig. 5.3).

(ii) **Bell mixture:** We consider a mixture of two Bell states, given by

$$\rho_{BM} = p|\phi^+\rangle\langle\phi^+| + (1-p)|\phi^-\rangle\langle\phi^-|,$$

where  $|\phi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$ ,  $|\phi^-\rangle = \frac{1}{\sqrt{2}}(|00\rangle - |11\rangle)$  and  $0 \leq p \leq 1$ . Numerical observations suggests that

$$\mathcal{I}_\alpha^\Gamma(\rho_{BM}) = \tilde{S}_\alpha^\Gamma\left(\rho_{BM} \parallel \frac{I}{4}\right),$$

for  $\alpha \geq \frac{2}{3}$  ( $\alpha \neq 1$ ). Hence, in this range of  $\alpha$ ,

$$\mathcal{I}_\alpha^R(\rho_{BM}) = 2 + \frac{1}{\alpha-1} \log [p^\alpha + (1-p)^\alpha]. \quad (5.37)$$

We have found numerically that if one performs measurement in the  $\{|0\rangle, |1\rangle\}$  basis, the relative entropy of the post-measurement state with  $\frac{I}{4}$  gives the Rényi classical correlation for the entire range of  $\alpha$ , i.e., for  $\alpha \in (\frac{1}{2}, 1) \cup (1, \infty)$ , and it is equal to unity for any  $p$  and  $\alpha$ . Hence for  $\alpha \geq \frac{2}{3}$  ( $\alpha \neq 1$ ),

$$\mathcal{D}_\alpha^R(\rho_{BM}) = 1 + \frac{1}{\alpha-1} \log [p^\alpha + (1-p)^\alpha]. \quad (5.38)$$

The linear quantum discord for this state is given by

$$\mathcal{D}_L(\rho_{BM}) = 8(p^2 - p) + 2. \quad (5.39)$$

Similarly,

$$\mathcal{D}_{max}(\rho_{BM}) = 1 + \log [\max\{p, 1-p\}]. \quad (5.40)$$

In Fig. 5.4, the Rényi quantum correlations for  $\rho_{BM}$  is depicted for different values of  $\alpha$ .

(iii) **Mixture of Bell state and a product state:** Consider the state given by

$$\rho_{BN} = p|\phi^+\rangle\langle\phi^+| + (1-p)|00\rangle\langle 00|.$$

The Rényi quantum correlation is calculated numerically, and in Fig. 5.5, we plot it for  $\rho_{BN}$ , for different values of  $\alpha$ .

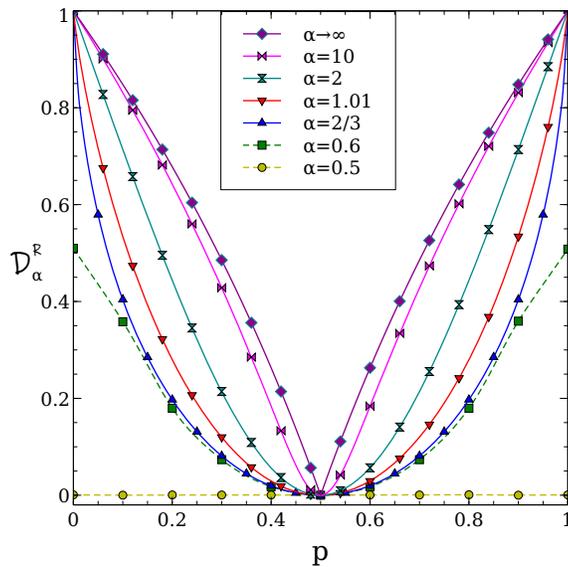


Figure 5.4: Rényi quantum correlation,  $\mathcal{D}_\alpha^R$ , with respect to  $p$ , of the Bell mixture,  $\rho_{BM} = p|\phi^+\rangle\langle\phi^+| + (1-p)|\phi^-\rangle\langle\phi^-|$ , for different values of  $\alpha$ . Both axes are dimensionless.

### 5.3.6 Sandwiched vs traditional relative entropies

Until now, in this section, we have used the sandwiched relative entropy distances to define the Rényi and Tsallis quantum correlations. We now briefly consider the traditional variety for defining quantum correlation, and discuss some of its implications. In the preceding subsections, we have observed anomalous behavior of the Rényi quantum correlation in the range  $\frac{1}{2} \leq \alpha < \frac{2}{3}$  for pure states, as well as in certain families of mixed states in the neighborhood of pure states. In these cases, we have, e.g., seen that the Bell states are not the maximally Rényi quantum correlated state for  $\alpha < \frac{2}{3}$  and at  $\alpha = \frac{1}{2}$ , i.e., for the min- entropy, all pure states have vanishing quantum correlations.

We can also define quantum correlations with the traditional relative Rényi and Tsallis entropies. The properties (1-4) discussed in Sec. 5.2, are also followed by both the traditional relative entropies [223], but the data processing inequality holds for  $\alpha \in [0, 1) \cup (1, 2]$  [224, 225, 226]. We can therefore define quantum correlation with traditional relative entropy distances for this range of  $\alpha$ . If we consider the traditional relative entropies, then we do not see any anomalous behavior of the Rényi quantum correlation. But from the traditional version of the relative Rényi entropy, we do not get the min- entropy. Moreover, in [195], the authors have argued that the sandwiched relative Rényi entropy is operationally relevant in the strong converse

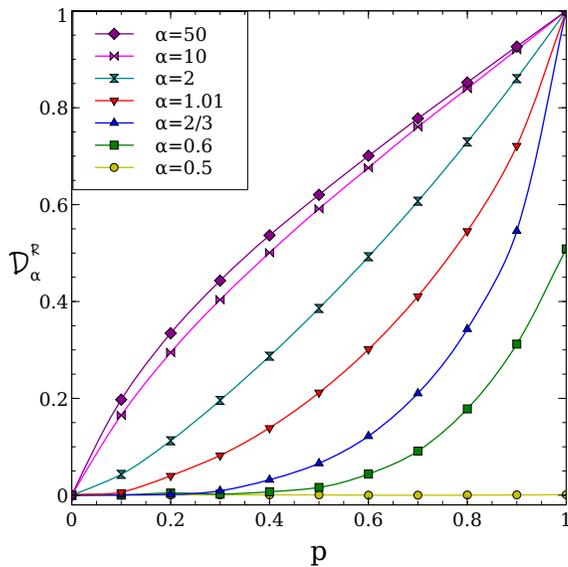


Figure 5.5: Rényi quantum correlation,  $\mathcal{D}_\alpha^R$ , with respect to  $p$ , of  $\rho_{BN} = p|\phi^+\rangle\langle\phi^+| + (1-p)|00\rangle\langle 00|$ , for different  $\alpha$ . Both axes are dimensionless.

problem of quantum hypothesis testing for  $\alpha > 1$ , but for  $\alpha < 1$ , the traditional version is more relevant from an operational point of view. The anomalous behavior of the quantum correlation with the sandwiched relative entropy distances seems to indicate that to define quantum correlation for  $\alpha < 1$ , the more appropriate candidates are the traditional relative entropies. Here we discuss about the traditional Rényi quantum correlation for two-qubit pure states and the Werner state.

**(i) Pure states:** Numerical observations similar to the case with the sandwiched variety, give us that the total correlation of a two-qubit pure state,  $|\psi_{AB}\rangle = \sum_{i=0}^1 \sqrt{\lambda_i} |i_A i_B\rangle$ , for traditional relative Rényi entropy, with  $\alpha \in (\frac{1}{2}, 1)$ , is given by

$$\mathcal{I}_\alpha^{TR}(|\psi_{AB}\rangle) = \min_{\{a\}} \frac{1}{\alpha - 1} \log \left[ \lambda a^{2(1-\alpha)} + (1-\lambda)(1-a)^{2(1-\alpha)} \right], \quad (5.41)$$

where  $0 \leq a \leq 1$ , and the value of  $a$  is obtained from the condition

$$\frac{1}{a} = \left( \frac{\lambda}{1-\lambda} \right)^{\frac{1}{1-2\alpha}} + 1. \quad (5.42)$$

The classical correlation in the traditional case is computed numerically. The numerical computation is performed by the same numerical recipe as mentioned in Sec. 5.3.4.

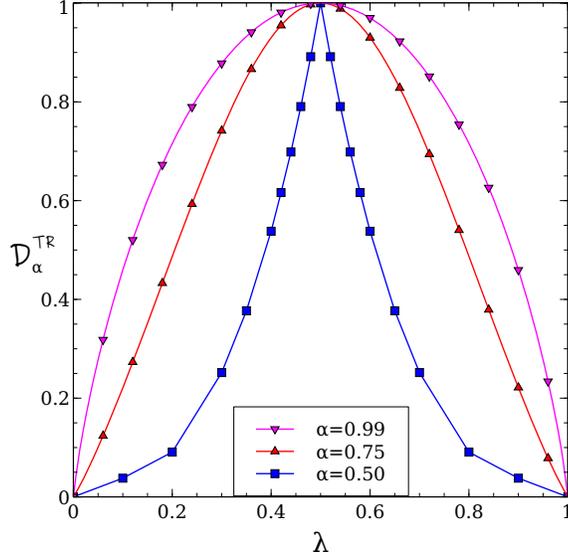


Figure 5.6: Traditional Rényi quantum correlation,  $\mathcal{D}_\alpha^{TR}$ , with respect to  $\lambda$ , of  $|\psi_{AB}\rangle = \sqrt{\lambda}|00\rangle + \sqrt{(1-\lambda)}|11\rangle$  for different  $\alpha$ . Both axes are dimensionless.

In Fig. 5.6, we have plotted the  $\mathcal{D}_\alpha^{TR}(|\psi_{AB}\rangle)$ , for different values of  $\alpha$ . No anomalous behavior can be seen, and the maximally entangled states have maximal quantum correlations.

**(ii) Werner states:** Like in the sandwiched version, exploiting the rotational invariance and symmetry of the Werner state, it can be shown analytically that the total correlation of the Werner state for the traditional relative Rényi entropy, for  $\alpha \in [\frac{1}{2}, 1)$ , is given by

$$\mathcal{I}_\alpha^{TR}(\rho_W) = 2 + \frac{1}{\alpha - 1} \log \frac{1}{4^\alpha} [(1 + 3p)^\alpha + 3(1 - p)^\alpha]. \quad (5.43)$$

The classical correlation of the Werner state is also measurement basis independent for the traditional version, like the sandwiched one. We get that the classical correlation, in this range, is given by

$$\mathcal{J}_\alpha^{TR}(\rho_W) = 2 + \frac{1}{\alpha - 1} \log \frac{1}{4^\alpha} [2(1 + p)^\alpha + 2(1 - p)^\alpha]. \quad (5.44)$$

The forms of the total and classical correlations, in this case, are equivalent to those in the sandwiched version. But here, the range of  $\alpha$  is different. Hence, for  $\alpha \in [\frac{1}{2}, 1)$ ,

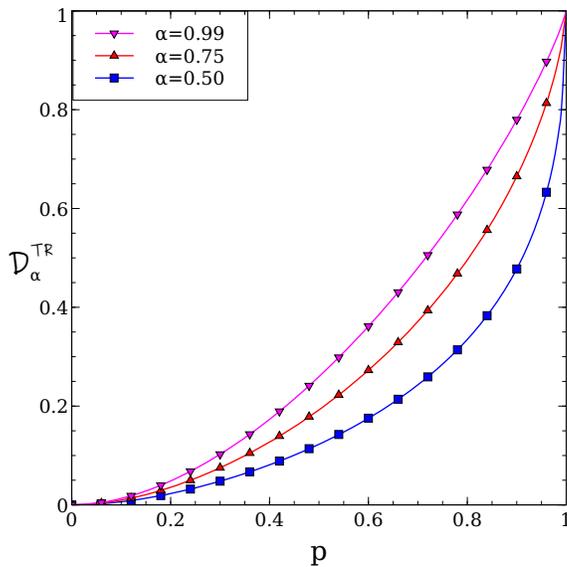


Figure 5.7: Traditional Rényi quantum correlation,  $\mathcal{D}_\alpha^{TR}$ , with respect to  $p$  of the Werner state,  $\rho_W = p|\psi^-\rangle\langle\psi^-| + (1-p)\frac{1}{4}I$ , for different  $\alpha$ . Both axes are dimensionless.

the traditional Rényi quantum correlation for the Werner state is given by

$$\mathcal{D}_\alpha^{TR}(\rho_W) = \frac{1}{\alpha - 1} \log \left[ \frac{(1 + 3p)^\alpha + 3(1 - p)^\alpha}{2(1 + p)^\alpha + 2(1 - p)^\alpha} \right]. \quad (5.45)$$

In Fig. 5.7, we have plotted the  $\mathcal{D}_\alpha^{TR}(\rho_W)$ , for different values of  $\alpha$ .

## 5.4 Application: Detecting criticality in quantum Ising model

In this section, we show that the Rényi and Tsallis quantum correlations can be applied to detect cooperative phenomena in quantum many-body systems. Let us consider a system of  $N$  quantum spin-1/2 particles, described by the one-dimensional quantum Ising model [227, 228, 229]. Such models can be simulated by using ultra-cold gases in a controlled way in the laboratories [36, 230, 231, 232, 233, 234, 235], and is also known to describe Hamiltonians of materials [236, 237, 238, 239]. The Hamiltonian for this system is given by

$$H = J \sum_{i=1}^N \sigma_i^x \sigma_{i+1}^x + h \sum_{i=1}^N \sigma_i^z, \quad (5.46)$$

where  $J$  is the coupling constant for the nearest neighbor interaction,  $\sigma$ 's are the Pauli spin matrices, and  $h$  represents the external transverse magnetic field applied across the system. Periodic boundary condition is assumed. The Hamiltonian can be diagonalized by applying Jordan-Wigner, Fourier, and Bogoliubov transformations [227]. At zero temperature, it undergoes a quantum phase transition (QPT) driven by the transverse magnetic field at  $\lambda \equiv \frac{h}{J} = \lambda_c \equiv 1$  [227]. Such a transition has been detected by using different order parameters [227, 228, 229, 240, 241], including quantum correlation measures like concurrence [34, 35], geometric measures [161, 242, 243, 244, 245], and quantum discord [166, 167, 168, 169].

We now investigate the behavior of the Rényi and Tsallis quantum correlations of the nearest neighbor density matrix (reduced density matrix of two neighboring spins) at zero temperature, near the quantum critical point. Note that we have reverted back to the sandwiched version of the relative entropies in this section. The nearest neighbor bipartite density matrix,  $\rho_{AB}$ , of the ground state of the Hamiltonian given by Eq. (5.46), represented by  $\rho_{AB}$ , can be written [227] in terms of the diagonal two-site correlators and the average magnetization in  $z$ -direction. The density matrix,  $\rho_{AB}$ , in the thermodynamic limit of  $N \rightarrow \infty$ , is given by

$$\rho_{AB} = \begin{pmatrix} \alpha_+ + \frac{M_z}{2} & 0 & 0 & \beta_- \\ 0 & \alpha_- & \beta_+ & 0 \\ 0 & \beta_+ & \alpha_- & 0 \\ \beta_- & 0 & 0 & \alpha_+ - \frac{M_z}{2} \end{pmatrix},$$

where  $\alpha_{\pm} = \frac{1}{4}(1 \pm T_{zz})$ ,  $\beta_{\pm} = \frac{T_{xx} \pm T_{yy}}{4}$  with  $T_{ij} = \text{Tr}(\sigma_i \otimes \sigma_j \rho_{AB})$  and  $M_z = \text{Tr}(\mathbb{I}_{\mathbb{A}} \otimes \sigma_z \rho_{AB})$ . The correlations and transverse magnetization, for the zero-temperature state, are given by [227]

$$\begin{aligned} T^{xx}(\lambda) &= G(-1, \lambda), \\ T^{yy}(\lambda) &= G(1, \lambda), \\ T^{zz}(\lambda) &= [M^z(\lambda)]^2 - G(1, \lambda)G(-1, \lambda), \end{aligned} \tag{5.47}$$

where

$$G(R, \lambda) = \frac{1}{\pi} \int_0^{\pi} d\phi \frac{(\sin(\phi R) \sin \phi - \cos \phi (\cos \phi - \lambda))}{\Lambda(\lambda)} \tag{5.48}$$

and

$$M^z(\lambda) = -\frac{1}{\pi} \int_0^\pi d\phi \frac{(\cos \phi - \lambda)}{\Lambda(\lambda)}. \quad (5.49)$$

Here

$$\Lambda(x) = \{\sin^2 \phi + [x - \cos \phi]^2\}^{\frac{1}{2}}, \quad (5.50)$$

and

$$\lambda = \frac{h}{J}. \quad (5.51)$$

Note that  $\lambda$  is a dimensionless variable. The Rényi and Tsallis quantum correlations are calculated for the state,  $\rho_{AB}$ , for different values of  $\alpha$ . In Fig. 5.8, we plot the Rényi quantum correlation as a function of  $\lambda$  for different values of  $\alpha$ . QPT corresponds to a point of inflexion in the  $\mathcal{D}_\alpha^r$  versus  $\lambda$  curve and  $\frac{d\mathcal{D}_\alpha^r}{d\lambda}$  diverges there. We claim that the derivatives of the Rényi (and the Tsallis) discords do diverge at the critical point. The seeming finiteness of the derivative at the critical point has to do with the finite spacing of the variable  $\lambda$ . To see this, we perform a finite-size scaling analysis of the full width at half maxima, of the peak that is obtained around the critical point for finite size (see Fig. 5.9).

This feature is distinctly different from the variation of the derivative of the quantum discord with respect to  $\lambda$  around the QPT point, which exhibits a point of inflexion at  $\lambda = 1$  [166, 167, 168, 169] (cf. [246]). It is only the second derivative of quantum discord with respect to  $\lambda$ , which diverges at the QPT point. This is an uncomfortable and intriguing feature of quantum discord, and is not shared by e.g. the concurrence at the same quantum critical point [34, 35]. Therefore it is advantageous to use the Rényi and Tsallis quantum correlations to detect phase transitions and other collective phenomena in quantum many body systems, in comparison to quantum discord.

**Finite-size scaling :** The Rényi and Tsallis quantum correlations are shown in Fig. 5.8 to detect phase transitions in infinite systems. Ultracold gas realization of such phenomena, however, can simulate the corresponding Hamiltonian for a finite number of spins [235]. The quantum Ising model, which has been briefly described earlier in this section, can also be solved for finite-size systems [227]. We calculate the quantum correlations of nearest neighbor spins for finite spin chains using both the Tsallis and Rényi entropies. We find that the quantum correlations detect the transition in finite-size systems too. Again, the transition point corresponds to points

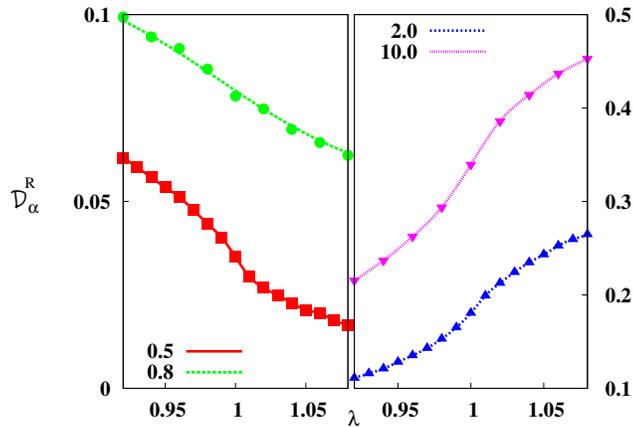


Figure 5.8: Detecting quantum phase transitions with Rényi quantum correlations. Rényi quantum correlation,  $\mathcal{D}_\alpha^R$ , with respect to  $\lambda$ , of the nearest neighbor bipartite density matrix at zero temperature, for different values of  $\alpha$ . The legends indicate the values of  $\alpha$ . Both axes are dimensionless. Near  $\lambda = 1$ ,  $\mathcal{D}_\alpha^R$  exhibits a point of inflexion and therefore, the derivative of  $\mathcal{D}_\alpha^R$  w.r.t.  $\lambda$  diverges at this point. This indicates the critical point in this transverse field Ising model.

of inflexion in the  $\mathcal{D}_\alpha^R$  versus  $\lambda$  curves, and narrow bell-shaped peaks in the  $\frac{d\mathcal{D}_\alpha^R}{d\lambda}$  versus  $\lambda$  curves, for different values of  $N$ . The bell-shaped curves become more narrow and peaked with the increase of number of spins. We perform a finite-size scaling analysis of full-width at half maxima,  $\delta_N$ , of the  $\frac{d\mathcal{D}_\alpha^R}{d\lambda}$  versus  $\lambda$  curves, and the scaling exponent is e.g. -0.36 for  $\mathcal{D}_2^R$  (see Fig. 5.9). The exponent is a measure of the rapidity with which the narrow bell-shaped peak tends to show a divergence with the increment in system size  $N$ . The log – log scaling between the size,  $N$ , and the width,  $\delta_N$ , clearly indicates divergence of the derivative at infinite  $N$ .

We also perform finite-size scaling analyses of the  $\lambda_c^N$ , the value of  $\lambda$  for which the derivatives of the Rényi (or Tsallis) quantum correlations with respect to  $\lambda$  has a maximum for a system of  $N$  spins, for several different values of  $\alpha$ , and obtain the corresponding scaling exponents. The exponent is a measure of the rapidity with which the QPT point,  $\lambda_c^N$ , in a finite size system of size  $N$ , approaches the QPT point,  $\lambda_c$ , of the infinite system, as a function of  $N$ .

Table 5.1 exhibits the scaling exponents for both  $\mathcal{D}_\alpha^R$  and  $\mathcal{D}_\alpha^T$  for some values of  $\alpha$ . It is found that for  $\alpha = 2$ , the scaling exponents are much higher for both  $\mathcal{D}_\alpha^R$  and  $\mathcal{D}_\alpha^T$  than any other known measures. In particular, the scaling exponents for transverse magnetization, fidelity, concurrence, quantum discord, and shared purity are respectively -1.69, -0.99, -1.87, -1.28, and -1.65 [34, 35, 247, 248, 249].

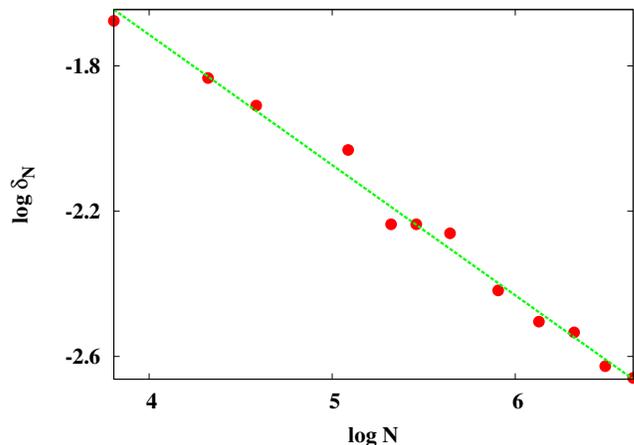


Figure 5.9: Scaling analysis of full-width at half maxima,  $\delta_N$ , for  $\mathcal{D}_2^R$ . Both axes are dimensionless.

Table 5.1: The scaling exponents for both  $\mathcal{D}_\alpha^R$  and  $\mathcal{D}_\alpha^T$  for some values of  $\alpha$ .

$\alpha$	$\mathcal{D}_\alpha^R$	$\mathcal{D}_\alpha^T$
2.0	-3.45	-3.74
10.0	-1.28	-0.87
50.0	-1.25	-2.74

## 5.5 Chapter summary

Quantum discord is a quantum correlation measure, belonging to the information-theoretic paradigm, and it has the potential to explain several quantum phenomena that cannot be explained by invoking the concept of quantum entanglement. In this chapter, we have defined quantum correlations with generalized classes of entropies, viz. the Rényi and the Tsallis ones. The usual quantum discord incorporates the von Neumann entropy in its definition. We have first defined the generalized mutual information in terms of sandwiched relative entropy distances. Using this definition of generalized mutual information, we have introduced the generalized quantum correlations, and have shown that they fulfill the intuitively satisfactory properties of quantum correlation measures. We have evaluated the generalized quantum correlations for pure states and some paradigmatic classes of mixed states.

As an application, we have found that the generalized quantum correlations can

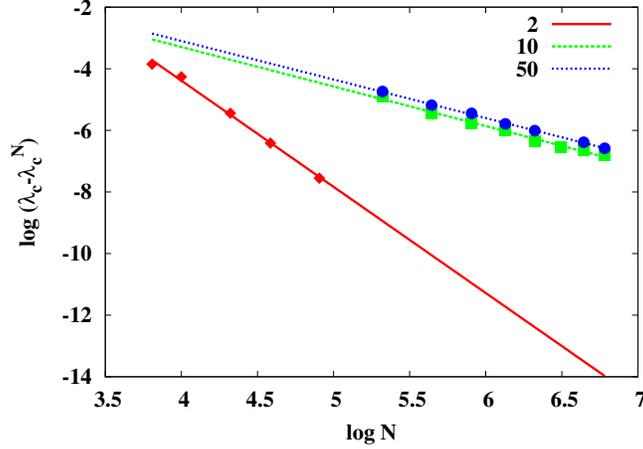


Figure 5.10: Scaling analysis of Rényi quantum correlation,  $\mathcal{D}_\alpha^R$ , for different values of  $\alpha$ , in the one-dimensional quantum Ising model. The legends indicate the values of  $\alpha$ . Both axes are dimensionless.

detect quantum phase transitions in the transverse quantum Ising model. Interestingly, a finite-size scaling analysis reveals that the scaling exponents obtained for the generalized quantum correlations can be significantly higher than the usual quantum discord as well as other order parameters, like transverse magnetization and concurrence, at the same critical point. This aspect can lead to the usefulness of these measures in quantum simulators in ultracold gas experiments, potentially realizing finite versions of quantum spin models. Moreover, while the derivative of the quantum discord provides only a point of inflexion at the quantum critical point, the derivative of the generalized quantum correlations defined here signals the same critical point via a divergence.

**N.B.** The results presented in this chapter are original. Using the definition and properties of generalized relative entropies derived in previous papers by other authors we define generalized mutual information or total correlation. Furthermore, we define classical correlation by maximizing the total correlation of the post measurement state. Thus, generalized quantum correlation can be defined by taking the difference between generalized total and classical correlation. After that, we have calculated generalized quantum correlation of bi-partite pure and paradigmatic classes of mixed states. We also show that generalized quantum correlation can detect quantum phase transition in transverse field quantum Ising model with better finite size scaling.

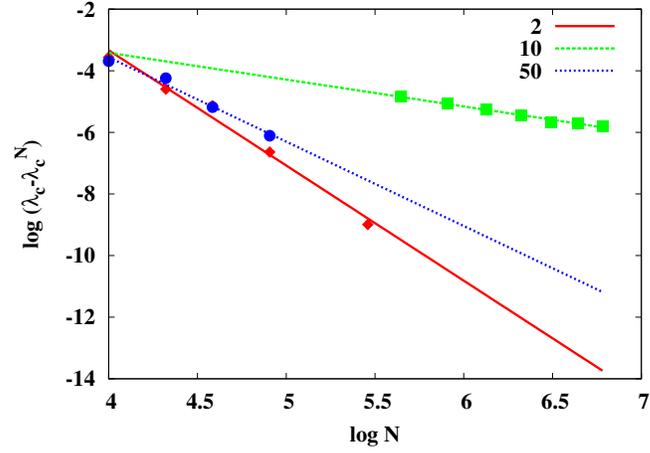


Figure 5.11: Scaling analysis of Tsallis quantum correlation,  $\mathcal{D}_\alpha^T$ , for different values of  $\alpha$ , in the one-dimensional quantum Ising model. The legends indicate the values of  $\alpha$ . Both axes are dimensionless.

The results of this chapter have been published in “*Quantum Correlation with Sandwiched Relative Entropies: Advantageous as Order Parameter in Quantum Phase Transitions*, A. Misra, A. Biswas, A.K. Pati, A. Sen De, U. Sen, *Phys. Rev. E* **91**, 052125 (2015).”

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# Quantum thermal machines and second law of thermodynamics

## 6.1 Introduction: Why quantum thermal machines?

The idea of quantum thermal machines (QTMs) have been around for years. What limits does quantum theory imposes to the performance of QTMs is an important yet difficult question. This fundamental issue has been of great interest in quantum thermodynamics for years. Most of models of QTMs are in agreement with the classic thermodynamic bounds. In contrast, there has been a increasing number of claims day-by-day that those bounds are not universal and can be surpassed using quantum resources [126, 127, 250, 251, 252, 253, 254, 255, 256, 257]. These claims necessitate cautious scrutiny of the working principle of the QTMs in a model independent approach and development of methods and techniques that can shed light on the laws of thermodynamics in the quantum regime. These are the main motivations that underlie the present study of QTMs. Majority of the theoretical models of QTMs proposed so far need experimental verification. This would not only advance the state-of-the-art quantum thermodynamics but can also bring revolution in the device miniaturization technology. As the size of the QTMs approaches much shorter scale we are inevitably bothered with quantum thermodynamic effects. That is why it is of utmost importance to study QTMs and formulate their thermodynamic performance limits. Designing principles that are needed for any application where efficiency, cooling rate, power and size constraints are crucial is becoming more relevant day by day. For example, with the increased number of micro-chips and transistors that produce heat while operating, the need of quantum refrigerators is

growing more than ever before. Some important but intriguing questions in the field of QTMs are as follows:

- How the QTMs differ from their classical counterparts in their working principle?
- What are the performance bounds of these QTMs?
- Does the Carnot bound on efficiency hold in QTMs?
- What is truly quantum in QTMs? What are the advantages that the quantumness of the QTMs brings?

These queries set the motivations for studying the QTMs in great detail.

## 6.2 Types of quantum thermal machines

QTMs can be classified mainly in two categories: (i) Reciprocating-cycle (ii) Continuous-cycle. Recently, a model of (iii) Hybrid-cycle heat machines has been introduced in Ref. [119].

- (i) *Reciprocating-cycle QTMs*: A reciprocating cycle consists of strokes in which the working system is alternately coupled to the hot and cold heat baths. Generally, it consists of four strokes, as in the case of the Carnot and Otto cycles, both of which consist two adiabatic strokes where the working medium is kept isolated from the thermal environments and a working piston drives the systems. There are also two heat transferring strokes in which the working medium is alternately coupled to either of the heat baths. In case of the Carnot cycle the strokes are isothermal, whereas isochores in the Otto cycle. They are also two-strokes engines [42] which consist of two parts. In one part the working medium may couple only to the hot bath, whereas the other may couple only to the cold bath. In the first stroke, both parts interact with their baths but may not necessarily equilibrate. In the second stroke, the two engine parts are separated from the baths and are connected to each other. A mutual unitary operation is applied on them in which work is extracted from.
- (ii) *Continuous-cycle QTMs*: In microscopic or nanoscale devices that operate obeying the laws of quantum mechanics, reciprocating cycles imposes crucial problems. On-off switching of the interaction between system and bath and non-adiabatic operation in quantum domain may affect the energy and heat transfer

during the cycles. These problems have motivated the study of shortcut to adiabaticity. However, in microscopic regime complete decoupling of system and bath may not be possible always. For these aforesaid reasons, it is important to consider continuous-cycle heat machines where the working medium remains continuously coupled with two heat baths in general, namely the hot and cold heat baths.

- *(iii) Hybrid-cycle QTMs:* Recently, a hybrid cycle model of heat machines has been introduced which is neither continuously coupled with heat bath nor completely decoupled from the baths also. The speed limits and performance bounds of this model have also been studied [119].

### 6.3 Quantum thermodynamic signatures

When we study QTMs, one important aspect is to identify the quantum advantages compared to their classical counterparts. One must differentiate between one machine which is exploiting the quantum effects and another one which is only operating quantum mechanically without exploiting quantum effects. For example, a machine is dealing with discrete energy levels but the working principle is exactly similar to the classical counterpart. This motivates the need of a witness of quantum thermodynamic signatures in QTMs. The idea is very similar to the witness of entanglement or Bell inequality, where one detects that some states are entangled or Bell nonlocal as they can pass certain test. Following the same manner, the possibility of a witness of quantum thermodynamic signatures has recently been addressed [42]. The main idea of Ref. [42] is to find an upper limit on the power of a machine which is operating classically. Therefore, violation of this bound can be witnessed as quantum thermodynamic signatures. In this article [42], minimal set of requirements have been made for a machine to be considered as classical.

The authors of Ref. [42] following their aforementioned approach has studied the four-stroke quantum Otto engine in detail. It has been established that a state independent bound can be posed on the power of the classical machine which is proportional to the duration of a complete single cycle as long as the product of the cycle time and energy scale is lower than some fixed limit. They demonstrate that there lies a regime where a quantum engine can outperform its classical counterpart. The similar results also holds for two-stroke and continuous cycle engines as they have shown that in the regime of weak coupling with the bath these cycle forms are

equivalent. The techniques and concepts used in quantum information theory have been useful for their study to find quantum thermodynamic signatures.

## 6.4 Quantum absorption refrigerators

In this section, we study one of the most remarkable QTM, self-contained quantum absorption refrigerator (QAR). QAR has been proposed in Ref. [258] of late inspired by the algorithmic cooling. This QAR provides cooling (or polarization) of one of the constituent qubits without any external control. As the QAR consists of only three qubits coupled with three baths locally, its working principle is very much simple. Considering the low dimensions of this machine, it is also argued to be smallest possible quantum refrigerator [258]. Despite its simplicity it promises significant applications in quantum technology, medical science, biology, chemical industry. This QAR could lead to breakthroughs in high-sensitivity NMR (Nuclear Magnetic Resonance) spectroscopy, development of scalable NMR quantum computers, quantum error correction protocols, etc. Apart from its promising applied importance, due to its simple working principle it can also be interesting to unravel quantum signatures in heat machines and a good testing bed for quantum thermodynamic phenomena. Efficiency of this model, general performance bounds, role of quantum resources like entanglement, coherence for better performance have been extensively demonstrated [117, 125, 127]. Recently, the importance of quantum entanglement to enhance the performance of the QAR has been pointed out [125]. Moreover, it has been shown that a little amount of coherence of the initial state of the QAR can enhance the performance significantly in the one-shot (transient) regime [117]. This QAR can also be utilized to generate steady entanglement in thermal environment. How to implement this model in the laboratory has also been proposed of late [259, 260]. Thus, the small quantum refrigerator has become a active field of study in recent times. Let us briefly discuss the model introduced in Ref. [258].

**The model:** The three qubits consisting the refrigerator are coupled to three different baths at different temperatures. The first qubit which is the object to be cooled, is coupled to the coldest bath at temperature  $T_C$ . The second qubit which takes energy from the first qubit and disposes into the environvent, is coupled to a hotter bath at temperature  $T_R$ . The third and final qubit which provides the free energy for refrigeration is couplped to the hottest bath at temperature  $T_H$ . Here  $T_C \leq T_R \leq T_H$ . Without loss of generality, the ground state energy of all the qubits are considered to be zero and the excited state energy of the  $i_{th}$  qubit is

$E_i$ , where  $i \in \{1, 2, 3\}$ . The free Hamiltonian of the combined system is  $H_0 = \sum_{i=1}^3 E_i |1\rangle_i \langle 1|$ . In thermal equilibrium the qubits are in the corresponding thermal states  $\tau_i = r_i |0\rangle \langle 0| + (1 - r_i) |1\rangle \langle 1|$ , where  $r_i = (1 + e^{-\beta_i E_i})^{-1}$  is the probability of the  $i_{th}$  qubit to be in the ground state. Here  $\beta_i$  is the inverse temperature  $1/T_i$ .

The qubits interact via the following interacting Hamiltonian  $H_{int} = g(|101\rangle \langle 010| + |010\rangle \langle 101|)$ . The interaction strength  $g$  is taken weak enough compared to the energy levels  $\{E_i\}$ , i.e.,  $g \ll E_i$ , so that the energy levels and the energy eigenstates of the combined system are almost unaltered and the temperature of the each qubit can be defined neglecting the interaction energy [258]. The total Hamiltonian of the combined system is given by

$$H = \sum_{i=1}^3 E_i |1\rangle_i \langle 1| + g(|101\rangle \langle 010| + |010\rangle \langle 101|). \quad (6.1)$$

As the qubits are coupled with heat baths at each time step there is finite probability that it will thermalize. Suppose,  $p_i$  is the probability density per unit time that the  $i_{th}$  qubit will thermalize back. Then the evolution of the combined system is given by the following master equation

$$\frac{\partial \rho}{\partial t} = -i[H_0 + H_{int}, \rho] + \sum_{i=1}^3 p_i (\tau_i \otimes Tr_i \rho - \rho). \quad (6.2)$$

It is necessary to mention that this master equation is valid only in the perturbative regime where  $p_i, g \ll E_i$  and  $p_i \ll 1$ . The thermalization of more than one qubit simultaneously is of second order in  $p_i$ 's and hence can be neglected. At any time instant the reduced density matrix of a single qubit is incoherent in energy eigenbasis and hence the temperature of the qubits can be defined locally. Here, the temperature defines the purity of the qubit being in the ground states.

**Transient cooling:** The study of transient quantum thermodynamics is certainly a topic of interest, both because in practical applications the transient regime might be the only accessible one, and quantum-driven enhancement of thermodynamic performance can, in certain cases, be better achieved at earlier stages of the dynamics, before the detrimental effects of Markovian baths kicks in. However, precise time control may be needed in transient cooling in QAR. We show that one can construct a QAR that provides refrigeration only in the transient regime [261]. The machine either does not provide cooling in the steady state, or the steady state is achieved after a long time. We propose a canonical form of qubit-bath interac-

tion parameters that facilitates the analysis of transient cooling without steady-state cooling. It has been observed that transient cooling without steady-state cooling is significantly better in terms of cooling power and efficiency. We also discuss how the performance of the transient refrigerator can be tuned by the temperature of the hot bath, and comment on the robustness of the phenomena against a small perturbation to the canonical form of the qubit-bath interaction parameters. We also show that with certain modification in the canonical form of qubit-bath interaction parameters which provides transient cooling without steady state cooling, it is possible to have fast and steady cooling towards the minimum steady state temperature where no precise time control is required to avail the transient cooling. We demonstrate our results for two separate models of thermalization. We perform a study of the dynamics of the bipartite and multipartite quantum correlations for both the models of thermalization. In the strong coupling regime, we find that the minimum achievable temperature of the refrigerated qubit and the minimal time to get optimal cooling can remain unchanged, for a significant region of the parameter space of the bath coupling strength as the initial dynamics is dictated by the coherent interaction among the qubits.

## 6.5 Quantum heat engines and Carnot bound

The Carnot bound can be achieved only by the ideal, reversible, infinitely-slow Carnot cycle and the efficiency of the same is given by

$$\eta_C = 1 - \frac{T_c}{T_h}, \quad (6.3)$$

where  $T_{c(h)}$  is the temperature of the cold (hot) heat bath. There is no common consensus regarding Carnot bound in quantum thermodynamics yet. Though it is considered universal in several models of quantum heat machines [41, 262, 263] it has also been contradicted many times [127, 251, 254, 255, 257]. These claims have been mainly based on the premise that there may be quantum thermodynamic resources, such as quantum coherence [255], squeez bath [126, 127, 253], or negative temperature of the bath [264] which may enhance work extraction or cooling ability of the quantum thermal machines. However, common consensus regarding Carnot bound in quantum thermodynamics is still lacking. In some models of quantum thermal machines, a cautious thermodynamic analysis has shown that the performance bounds do not surpass the Carnot limit [263]. As the thermodynamic consequences

of quantum effects, such as coherence, entanglement as well as the work extraction or cooling power of quantum states, are still not completely understood yet, such potential quantum resources must be examined further, considering all the energy sources and work cost. Recently, in Ref. [265] it has been argued that a engine operating in a Carnot cycle cannot surpass the classical Carnot bound even exploiting the quantum resources of the working fluid provided it is operating in contact with thermal baths. It has been also pointed out that energy is needed to maintain a nonequilibrium state which is in contact with thermal bath, following the concepts of stochastic thermodynamics.

In this chapter, with a motivation to probe the Carnot bound further we study the Carnot engine in the context of generalized entropy, namely the Rényi entropy. Our aim is to understand the physical reason that underlie the Carnot statement of the second law of thermodynamics. Towards this aim, we first establish the quantum thermodynamics based on the Rényi entropy. Then, we investigate the Carnot statement of second law of thermodynamics in this generalized thermodynamics. We also study the Clausius inequality which is the precursor to the Carnot statement.

## 6.6 Generalized thermodynamics

The foundation of modern quantum thermodynamics research [108, 265, 266, 267, 268] is based on the von Neumann entropy. The maximum entropy principle [17, 18] with mean energy constraint gives rise to the Gibbs state which plays an important role in recent works on thermal operations and thermodynamical laws [31, 32, 33, 269]. In this way the theory of quantum thermodynamics is developed based on von Neumann entropy. It is worth noting that the Gibbs states obtained consist of the exponential probability distributions. However, there are numerous physical systems which cannot be described by the Gibbsian exponential probability distribution and thereby inevitably needs the power law distributions [270]. Precisely, the physics and thermodynamics of fractal and multifractal systems found in grain boundaries in metals, fluid dynamics, percolation, diffusion limited aggregation systems, DNA sequences are described suitably by using the Rényi entropy [189, 270, 271]. Moreover, it is shown that Rényi entropy and its relative versions [272] are indispensable in defining the second laws of quantum thermodynamics in microscopic regime [31, 33].

It has been known for about half a century, Rényi entropy [171, 273] is endowed with all the necessary requirements for describing thermodynamics. Only recently [274] the maximum entropy state with fixed energy was formulated and derived, giv-

ing rise to the Rényi thermal state indexed by the Rényi parameter,  $\alpha$ . When  $\alpha \rightarrow 1$ , one obtains all the von Neumann results. We construct here a complete theory of thermodynamics on par with the von Neumann theory. This generalization enlarges the scope of another facet of thermodynamics with several second laws [31] and also the Gibbs preserving maps giving rise to Rényi thermal state preserving maps [269]. Another important outcome of this formalism is in establishing the *universality* of second laws of thermodynamics stated as based on the Carnot statement. Furthermore, exploiting the data processing inequalities [272] obeyed by the two versions of Rényi relative entropies, the Clausius inequality is shown to hold. We thus find that the Rényi entropy and its relative versions are the ingredients for establishing the second laws of thermodynamics in this chapter.

### 6.6.1 Generalized first law of thermodynamics

The Gibbs state, which is the equilibrium state, is obtained by maximizing the von Neumann entropy with a fixed internal energy. The maximum entropy (MaxEnt) principle [17, 18] is the underlying principle for such kind of equilibrium condition. It suggests that changing the definition of entropy functional, as well as the form of internal energy, gives rise to a new equilibrium state and hence a new theory of thermodynamics.

The Rényi entropy [273, 275], which is a generalization of the von Neumann entropy, is given by  $S_\alpha(\rho) = \frac{1}{1-\alpha} \ln(\text{Tr}\rho^\alpha)$ , for a density matrix  $\rho$  and  $\alpha \in (0, 1) \cup (1, \infty)$ . Note that we do not use the superscript “ $R$ ” to denote the Rényi entropy, as unlike chapter 5, here we only deal with the Rényi version of the generalized entropies. Moreover, we take natural “logarithm” with standard base throughout the chapter. The Rényi internal energy [274] of  $\rho$  is defined as  $U_\alpha = \text{Tr}[\rho^\alpha H]/\text{Tr}\rho^\alpha$ , where  $H$  is the Hamiltonian of the system. Note that  $S_\alpha(\rho)$  and  $U_\alpha$  reduce to von Neumann entropy,  $S(\rho) = -\text{Tr}(\rho \ln \rho)$  and internal or average energy  $U = \text{Tr}(\rho H)$  respectively, for  $\alpha \rightarrow 1$ . The thermal equilibrium state for the Rényi entropy can be derived using MaxEnt principle, i.e., maximizing  $S_\alpha(\rho)$  subject to a fixed internal energy  $U_\alpha$ , and is given by [274]

$$\rho_{T\alpha} = \frac{1}{Z_\alpha} [1 - (1 - \alpha)\beta(H - U_{T\alpha})]^{1/(1-\alpha)}. \quad (6.4)$$

Here,  $Z_\alpha = \text{Tr} \left[ \{1 - (1 - \alpha)\beta(H - U_{T\alpha})\}^{1/(1-\alpha)} \right]$  and  $U_{T\alpha} = \text{Tr}[\rho_{T\alpha}^\alpha H]/\text{Tr}\rho_{T\alpha}^\alpha$ . The inverse temperature  $\beta = 1/T$  (with the Boltzmann constant is set to unity) is defined

as  $\beta = \frac{\partial S_\alpha(\rho_{T\alpha})}{\partial U_{T\alpha}}$  which is a function of  $\alpha$ . Additionally the constraint  $[1 - (1 - \alpha)\beta(H - U_{T\alpha})] \geq 0$  is imposed to ensure the positive semi-definiteness of the thermal density matrix. Note that the Rényi thermal state reduces to the Gibbs state when  $\alpha \rightarrow 1$ . It should be noted that, similar to the Gibbs thermal state, one can also prepare Rényi thermal states, Eq. (6.4), via environmental interaction and relaxation. A natural testbed for this would be multifractal systems among others [189]. Further, the equilibrium *free energy* can be identified as  $F_{T\alpha} = U_{T\alpha} - TS_\alpha(\rho_{T\alpha})$  [274]. This general feature of the MaxEnt is independent of the choice of the form of the density matrix [276].

Now, we derive the generalized *first law of thermodynamics* considering the change in equilibrium Rényi internal energy as

$$dU_{T\alpha} = \frac{\text{Tr}[d\rho_{T\alpha}^\alpha(H - U_{T\alpha})]}{\text{Tr}\rho_{T\alpha}^\alpha} + \frac{\text{Tr}(\rho_{T\alpha}^\alpha dH)}{\text{Tr}\rho_{T\alpha}^\alpha}. \quad (6.5)$$

Under quasistatic isothermal process, the change in the entropy of the equilibrium state is  $\beta \text{Tr}[d\rho_{T\alpha}^\alpha(H - U_{T\alpha})]/\text{Tr}\rho_{T\alpha}^\alpha$ . Thus, the term  $\text{Tr}[d\rho_{T\alpha}^\alpha(H - U_{T\alpha})]/\text{Tr}\rho_{T\alpha}^\alpha$  can be identified as the heat exchanged. Moreover,  $\text{Tr}(\rho_{T\alpha}^\alpha dH)/\text{Tr}\rho_{T\alpha}^\alpha$  can be identified as the work done on the system,  $dW_{T\alpha}$ , where it is considered to be the change in internal energy due to the change in an extensive parameter. Hence, the Eq. (6.5) can be recast as

$$dU_{T\alpha} = dQ_{T\alpha} + dW_{T\alpha}. \quad (6.6)$$

This is the quantitative statement of the first law of thermodynamics following generalized theory of statistical mechanics based on the Rényi entropy. For a quasistatic isothermal process  $dW_{T\alpha} = dF_{T\alpha}$ , i.e., the infinitesimal change in the equilibrium free energy is the accessible work in the process. Therefore, for quasistatic isothermal processes we have

$$dU_{T\alpha} = dS_\alpha(\rho_{T\alpha})/\beta + dF_{T\alpha}. \quad (6.7)$$

Note that the generalized first law of thermodynamics reduces to the well known first law of quantum thermodynamics (based on the von Neumann entropy) when  $\alpha \rightarrow 1$ .

## 6.6.2 Free energy for nonequilibrium states

Till this point we deal only with equilibrium thermodynamics. What if the system is away from equilibrium? In what follows, we study the thermodynamics of nonequilibrium states using the Rényi relative entropy with a motive to answer this question.

For a nonequilibrium quantum state  $\rho_N$ , which may be a solution of a dynamical master equation (such as in Ref. [277]), the Rényi entropy can be written as

$$S_\alpha(\rho_N) = S_\alpha(\rho_{T\alpha}) - S_\alpha(\rho_N \parallel \rho_{T\alpha}) + \Delta_\alpha, \quad (6.8)$$

where  $S_\alpha(\rho \parallel \sigma) = \frac{1}{\alpha-1} \ln \text{Tr}[\rho^\alpha \sigma^{1-\alpha}]$  is the “traditional Rényi relative entropy” between two quantum states  $\rho$  and  $\sigma$ , and  $\Delta_\alpha = \frac{1}{\alpha-1} \ln [1 - \beta(1-\alpha)(U_{N\alpha} - U_{T\alpha})]$  with  $U_{N\alpha} = \text{Tr}[\rho_N^\alpha H]/\text{Tr}[\rho_N^\alpha]$  being the Rényi internal energy of  $\rho_N$ . Now we have

$$S_\alpha(\rho_N) = \beta [U_{N\alpha} - (F_{T\alpha} + \beta^{-1} S_\alpha(\rho_N \parallel \rho_{T\alpha}))] + \Delta'_\alpha, \quad (6.9)$$

where  $\Delta'_\alpha = [\beta(U_{T\alpha} - U_{N\alpha}) + \Delta_\alpha]$ . One can easily check that  $\Delta'_\alpha \rightarrow 0$  when  $\alpha \rightarrow 1$  and the above equation reduces to the usual von Neumann case. Thus, for nonequilibrium states we have  $S_\alpha(\rho_N) = \beta(U_{N\alpha} - \tilde{F}_{N\alpha})$ , where

$$\tilde{F}_{N\alpha} = F_{T\alpha} + \beta^{-1} (S_\alpha(\rho_N \parallel \rho_{T\alpha}) - \Delta'_\alpha), \quad (6.10)$$

is the modified free energy of the nonequilibrium state.

Considering again a quasistatic isothermal process, the change in entropy of the stationary nonequilibrium state is given by

$$dS_\alpha(\rho_N) = \beta(dU_{N\alpha} - d\tilde{F}_{N\alpha}) = \beta[dQ_\alpha - dQ_{hk\alpha}], \quad (6.11)$$

where  $dQ_\alpha = \text{Tr}[d\rho_N^\alpha (H - U_{N\alpha})]/\text{Tr}\rho_N^\alpha$ , and  $dQ_{hk\alpha} = d\tilde{F}_{N\alpha} - dW_\alpha$ , with  $dW_\alpha = \text{Tr}(\rho_N^\alpha dH)/\text{Tr}\rho_N^\alpha$ .  $dQ_\alpha$  is the total heat exchanged during the isothermal process and  $dQ_{hk\alpha}$  can be identified as the *house-keeping* heat, in the same spirit as in stochastic thermodynamics [26, 265, 278, 279, 280], which is used to maintain the nonequilibrium state away from thermal equilibrium. Now, for isothermal quasistatic processes in a generic quantum system, the Eq. (6.6) can be recast as

$$dU_{N\alpha} = dQ_{ex\alpha} + dW_{ex\alpha} = \beta^{-1} dS_\alpha(\rho_N) + d\tilde{F}_{N\alpha}, \quad (6.12)$$

where we denote excess heat as  $\tilde{d}Q_{ex\alpha} = \tilde{d}Q_\alpha - \tilde{d}Q_{hk\alpha}$  and extractable work as  $\tilde{d}W_{ex\alpha} = \tilde{d}Q_{hk\alpha} + \tilde{d}W_\alpha = \tilde{d}\tilde{F}_{N\alpha}$ . It is worth noticing that the notions of accessible work and the heat that results in entropy change, drastically differ from the equilibrium case (cf. Eq. (6.6)). Later, we will see that the notions of heat exchanged and accessible work in Eq. (6.6) are not compatible in nonequilibrium scenario if the thermodynamical laws have to be valid in that case too.

The above analysis can also be carried by using the “sandwiched Rényi relative entropy” [193, 194], which is defined as  $\tilde{S}_\alpha(\rho \parallel \sigma) = \frac{1}{\alpha-1} \ln \text{Tr}[\{\sigma^{\frac{1-\alpha}{2\alpha}} \rho \sigma^{\frac{1-\alpha}{2\alpha}}\}^\alpha]$ , between two quantum states  $\rho$  and  $\sigma$ . As the sandwiched Rényi relative entropy incorporates the noncommutivity of the quantum states, unlike the traditional version, it is intuitively satisfactory to expect that the former can outperform the latter to unravel quantum features. Indeed, the profound advantages of the sandwiched relative entropy in studying classical capacity of a quantum channel [193], witnessing entanglement [196, 281], quantum phase transitions [282], nonasymptotic quantum information theory [197, 198, 201], etc, have been noticed very recently. Therefore, it is quite legitimate to extend the study of nonequilibrium quantum thermodynamics exploiting the sandwiched Rényi relative entropy.

The entropy of a nonequilibrium state  $\rho_N$  can also be written as

$$S_\alpha(\rho_N) = S_\alpha(\rho_{T\alpha}) - \tilde{S}_\alpha(\rho_N \parallel \rho_{T\alpha}) + \tilde{\Delta}_\alpha, \quad (6.13)$$

where  $\tilde{\Delta}_\alpha = \frac{1}{\alpha-1} \ln [\text{Tr}(A^{1/2\alpha} \rho A^{1/2\alpha})^\alpha / \text{Tr}(\rho^\alpha)]$  and  $A = [1 - (1 - \alpha)\beta(H - U_{T\alpha})]$ . Thus, we have  $S_\alpha(\rho_N) = \beta(U_{N\alpha} - \mathcal{F}_{N\alpha})$ , where

$$\mathcal{F}_{N\alpha} = F_{T\alpha} + T \left( \tilde{S}_\alpha(\rho_N \parallel \rho_{T\alpha}) - \tilde{\Delta}'_\alpha \right), \quad (6.14)$$

is the modified free energy and  $\tilde{\Delta}'_\alpha = [\beta(U_{T\alpha} - U_{N\alpha}) + \tilde{\Delta}_\alpha]$ . Again  $\tilde{\Delta}'_\alpha \rightarrow 0$  when  $\alpha \rightarrow 1$  and it recovers the von Neumann case. The nonequilibrium entropy change and the internal energy change for a quasistatic isothermal process can be derived following the same way as in the context of Eqs. (6.11) and (6.12). Moreover, here also the change in the modified free energy  $d\mathcal{F}_{N\alpha}$  can be distinguished as the accessible work in a quasistatic isothermal process.

### 6.6.2.1 Free energy is minimum for thermal states

The free energy of an arbitrary quantum state is larger than that of a thermal equilibrium state, i.e.,  $\tilde{F}_{N\alpha} > F_{T\alpha}$ , for any  $\alpha$ . This follows from the Eq.

$$\tilde{F}_{N\alpha} = F_{T\alpha} + T(S_{\alpha}(\rho_N \parallel \rho_T) - \Delta'_{\alpha}), \quad (6.15)$$

$S_{\alpha}(\rho_N \parallel \rho_T) \geq 0$  and  $\Delta'_{\alpha} \leq 0$ . The first inequality,  $S_{\alpha}(\rho_N \parallel \rho_T) \geq 0$ , is due to the positivity of the Rényi relative entropy. The negativity of the latter quantity, can be shown by demanding the condition  $\beta(\alpha - 1)(U_{N\alpha} - U_{T\alpha}) > -1$ , which is the cut off condition of consistent probabilistic interpretation of Rényi thermal state, and the inequality  $\ln(1 + x) \leq x$  for all  $x > -1$ . Thus, confirming the known result that MaxEnt state implies minimum free energy.

### 6.6.3 Second laws of thermodynamics based on Carnot statement

Now let us address the validity of second laws of thermodynamics based on the Carnot statement [283] of the second law. Consider a four stroke Carnot engine operating between two reservoirs (heat baths), the hot and the cold with the temperatures  $T_h$  and  $T_c$  respectively (see Fig. 6.1). The baths consist of the Rényi thermal states with temperatures being  $\alpha$  dependent. We find the efficiency of this engine using the notions of accessible work and heat exchange which is responsible for entropy production developed earlier. In the first step, the system absorbs  $Q_{ex,1} = T_h[S_{\alpha}(\gamma_2, T_h) - S_{\alpha}(\gamma_1, T_h)]$ , amount of excess heat in a isothermal process at temperature  $T_h$ , from the the hot reservoir and the excess work  $W_{ex,1}$ , done by the system during the process is given by  $\tilde{F}_{N\alpha}(\gamma_1, T_h) - \tilde{F}_{N\alpha}(\gamma_2, T_h)$ , where  $\gamma$  is the external parameter which is varied during the processes throughout the cycle. The system performs  $W_{ex,2}$  work adiabatically in the second step and as it is an isentropic process the work done is at the cost of internal energy. As a consequence of performing work adiabatically, the temperature of the system falls down to  $T_c$ . Therefore in this step,  $W_{ex,2} = \tilde{F}_{N\alpha}(\gamma_2, T_h) - \tilde{F}_{N\alpha}(\gamma_3, T_c) + (T_h - T_c)S_{\alpha}(\gamma_2, T_h)$ . During the third step the work is actually done on the system in a isothermal process at temperature  $T_c$  and the system releases some excess heat. The heat absorbed,  $Q_{ex,3}$  and the work done,  $W_{ex,3}$  by the system are given by  $T_c[S_{\alpha}(\gamma_4, T_c) - S_{\alpha}(\gamma_3, T_c)]$  and  $\tilde{F}_{N\alpha}(\gamma_3, T_c) - \tilde{F}_{N\alpha}(\gamma_4, T_c)$ , respectively. Note that we are always expressing the work done and heat absorbed by the system and we follow the same convention for all

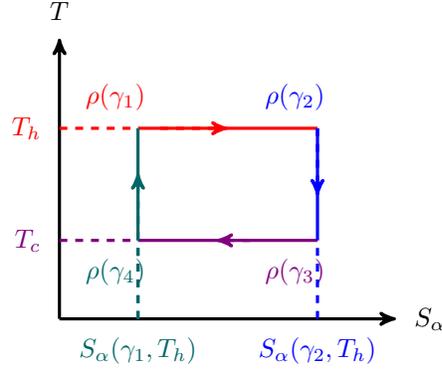


Figure 6.1: Schematic of Carnot cycle.  $1 \rightarrow 2$  and  $3 \rightarrow 4$  are the two isothermal steps at constant temperature  $T_h$  and  $T_c$  respectively.  $2 \rightarrow 3$  and  $4 \rightarrow 1$  are the adiabatic, isentropic steps. The different steps are performed by varying an external parameter  $\gamma$ .

the four steps. In the fourth step, work is again performed on the system adiabatically. As a result, the temperature of the system increases from  $T_c$  to  $T_h$  and the system is returned back to its initial state. The work done by the system is given by  $W_{ex,4} = \tilde{F}_{N\alpha}(\gamma_4, T_c) - \tilde{F}_{N\alpha}(\gamma_1, T_h) - (T_h - T_c)S_\alpha(\gamma_1, T_h)$ . Now, the Carnot efficiency which is the ratio of total work done by the system and the heat absorbed by the system in the first step, is given by

$$\eta_C = \frac{W_{ex,1} + W_{ex,2} + W_{ex,3} + W_{ex,4}}{Q_{ex,1}} = 1 - \frac{T_c}{T_h}, \quad (6.16)$$

for arbitrary stationary quantum states. Thus, the Carnot efficiency matches with the one in classical thermodynamics. Importantly, the Carnot efficiency remains the same for both the traditional and sandwiched Rényi relative entropies. Since we consider arbitrary quantum states, it can be stated that the quantum correlation or coherence cannot be exploited to enhance the efficiency beyond the classical Carnot limit. Therefore, if we account the accessible work and excess heat properly then *efficiency of any quantum engine undergoing a Carnot cycle is bounded above by  $\eta_C$* . Thus, the Carnot statement of the second law of thermodynamics has been followed universally in the Rényi formulation, in parallel with the Gibbsian formulation of the same [265].

Note that the identification of heat exchange and accessible work in nonequilibrium scenario which results in accounting the accessible work by change in free energy (internal energy minus temperature times entropy) in isothermal processes, is consistent with the Carnot statement of the second law of thermodynamics. Thus,

the form of free energy

$$F_\alpha = U_\alpha - TS_\alpha \quad (6.17)$$

is valid (from operational viewpoint, like work extraction) in nonequilibrium scenario too, where  $T$  is the temperature of the corresponding heat bath (the relevant one, depending on the protocol). One may note that both the free energies in Eqs. (6.10) and (6.14) are the same, i.e.,  $\mathcal{F}_{N\alpha} = \tilde{F}_{N\alpha}$ , and given by the aforementioned form. It reflects that the form of the free energy of a nonequilibrium state is independent of the relative entropy “distances”, though the definition of free energy of the same is based on its “distance” from the equilibrium one. A priori there is no reason why this form of free energy should be valid beyond equilibrium where the notion of temperature is not defined even. But this definition is consistent with the second law of thermodynamics. Moreover, as the free energy of the generalized thermal state is minimum among all the quantum states for all  $\alpha$  and the change in free energy is the accessible work in an isothermal process, *it is not possible to extract work from a single heat bath*, which is another aspect of the second laws of thermodynamics. Thus, the apparent *universality* of the second law of thermodynamics is a consequence of the *form invariance* of the free energy. Note that this form of the free energy emerges naturally from the MaxEnt principle.

Interestingly, the apparently different forms of free energies discussed in Ref. [265] and Ref. [108] are indeed equivalent and is a special case ( $\alpha \rightarrow 1$ ) of the generalized free energy given in Eq. (6.17). In Ref. [108], it is shown that if there exists any protocol by which one can extract more work than the free energy difference, then there would surely be a violation of the second law of thermodynamics. Similarly, in Ref. [265], it is shown that the maximum extractable work, in any step in a Carnot cycle, has to be restricted by the free energy difference, if it has to be consistent with the second law of thermodynamics. Therefore, it is evident that the validity of the second laws of thermodynamics is a consequence of the form invariance of the free energy when it is derived from the MaxEnt principle which sets the condition for equilibrium.

#### 6.6.4 Second laws based on Clausius inequality

The second laws of thermodynamics can further be substantiated in terms of the Clausius inequality in the Rényi formalism. Consider nonequilibrium states which are close to the thermal equilibrium state, such that  $U_{N\alpha} \approx U_{T\alpha}$ , i.e., the difference of

the internal energies is small. Moreover, consider infinitesimal change of the nonequilibrium state  $\rho_N$  by Rényi thermal state preserving map  $\Upsilon$ , i.e.,  $\rho_N \xrightarrow{\Upsilon} \rho_N + \delta\rho$ , where  $\Upsilon$  is a completely positive trace preserving (CPTP) map that keeps the Rényi thermal state  $\rho_{T\alpha}$  intact. As  $\rho_N$  is close to  $\rho_{T\alpha}$  and  $\Upsilon$  introduces infinitesimal change in  $\rho_N$ , therefore,  $\rho_N + \delta\rho$  is also close to  $\rho_{T\alpha}$ . Now, from Eq. (6.8), the variation in the traditional Rényi relative entropy becomes  $\delta S_\alpha(\rho_N \parallel \rho_{T\alpha}) = -\delta S_\alpha(\rho_N) + \delta\Delta_\alpha$ , where  $\delta S_\alpha(\rho_N \parallel \rho_{T\alpha}) = S_\alpha(\Upsilon[\rho_N] \parallel \Upsilon[\rho_{T\alpha}]) - S_\alpha(\rho_N \parallel \rho_{T\alpha})$ . Using the data processing inequality [284, 285] for the traditional relative Rényi entropy which says that  $\delta S_\alpha(\rho_N \parallel \rho_{T\alpha}) \leq 0$ , for  $\alpha \in [0, 2]$ , we show that

$$\beta \delta Q_{total} \leq \delta S_\alpha(\rho_N). \quad (6.18)$$

This is nothing but the well known Clausius inequality. Also exploiting the data processing inequality for the sandwiched relative Rényi entropy for  $\alpha \in [\frac{1}{2}, \infty)$  [194, 209, 210], we show that the Clausius inequality holds for  $\alpha \in [0, \infty)$ , where  $\rho_{T\alpha}, \rho_N$  and  $\delta\rho$  are mutually commuting

#### 6.6.4.1 Clausius inequality in $\alpha \in [0, 2]$

Consider an infinitesimal change in the density matrix of the system,  $\rho_N \rightarrow \Upsilon[\rho_N] = \rho_N + \delta\rho$  via a CPTP map that keeps the Rényi thermal state intact. We dub such maps as Rényi thermal state preserving maps. The change in the traditional Rényi relative entropy under such maps, is given by

$$\begin{aligned} \delta S_\alpha(\rho_N \parallel \rho_T) &= S_\alpha(\Upsilon[\rho_N] \parallel \rho_T) - S_\alpha(\rho_N \parallel \rho_T) \\ &= -\delta S_\alpha(\rho_N) + \delta\Delta_\alpha, \end{aligned} \quad (6.19)$$

where

$$\begin{aligned} \delta\Delta_\alpha &= \frac{-\beta(1-\alpha)}{(\alpha-1)[1-\beta(1-\alpha)(U_{N\alpha}-U_{T\alpha})]} \delta(U_{N\alpha}-U_{T\alpha}) \\ &= \frac{-\beta(1-\alpha)}{(\alpha-1)[1-\beta(1-\alpha)(U_{N\alpha}-U_{T\alpha})]} \delta U_{N\alpha} \\ &= \frac{\beta}{[1-\beta(1-\alpha)(U_{N\alpha}-U_{T\alpha})]} \left( \frac{\text{Tr}[\delta\rho_N^\alpha(H-U_{N\alpha})]}{\text{Tr}(\rho_N^\alpha)} \right) \\ &= \beta \delta Q_{total}(1+\beta(1-\alpha)(U_{N\alpha}-U_{T\alpha})). \end{aligned} \quad (6.20)$$

$$\approx \beta \delta Q_{total}, \quad (6.21)$$

We have used the fact that  $\delta Q_{total} = \delta U_N$ , as Hamiltonian  $H$  remains unchanged and  $(U_{N\alpha} - U_{T\alpha})$  is very small. Thus, we have

$$\delta S_\alpha(\rho_N \parallel \rho_T) = -\delta S_\alpha(\rho_N) + \beta \delta Q_{total}. \quad (6.22)$$

Now, using the data processing inequality for traditional Rényi relative entropy [284, 285],  $S_\alpha(\Upsilon[\rho_N] \parallel \Upsilon[\rho_T]) \leq S_\alpha(\rho_N \parallel \rho_T)$ , for  $\alpha \in [0, 2]$ , we have

$$-\delta S_\alpha(\rho_N) + \beta \delta Q_{total} \leq 0. \quad (6.23)$$

Therefore, we have  $\delta S_\alpha(\rho_N) \geq \beta \delta Q_{total}$  for  $\alpha \in [0, 2]$ , which is a statement of the second law of thermodynamics in terms of Clausius inequality. The Clausius inequality for transformations under unital maps near the equilibrium was shown in Ref. [285] for  $\alpha \in (0, 2]$ , by a different approach. However, the Clausius inequality derived above applies to the Rényi thermal state preserving operations. Clausius inequality has also been shown in Ref. [266, 267, 268] for von Neumann case.

Notice that if  $\rho_T$ ,  $\rho_N$  and  $\delta\rho$  are mutually commuting then the traditional relative entropies can be replaced by the sandwiched ones in Eq. (6.22) and following the data processing inequality for sandwiched relative entropies [193, 194] which holds for  $\alpha \in [\frac{1}{2}, \infty)$ , the Clausius inequality can be established for  $\alpha \in [0, \infty)$  for commuting case. Remarkably the Clausius inequality implies that the free energy is a monotone under Rényi thermal state preserving maps, when the Hamiltonian is kept fixed. This can also be seen from Eq. (6.10), when  $U_{N\alpha} \approx U_{T\alpha}$ .

#### 6.6.4.2 Clausius inequality for noncommuting states for $\alpha > 2$

If  $\rho_N + \delta\rho$ ,  $\rho_N$  and  $\rho_T$  are mutually commuting, then both  $\tilde{S}_\alpha(\rho_N + \delta\rho \parallel \rho_T)$  and  $\tilde{S}_\alpha(\rho_N \parallel \rho_T)$  vanish independently to the first order for our case of interest, i.e., for close by  $\rho_N$  and  $\rho_T$  and for  $\alpha \in [\frac{1}{2}, \infty)$ , we have

$$\delta \tilde{S}_\alpha(\rho_N \parallel \rho_T) = -\delta S_\alpha + \beta \delta U_{N\alpha} + \delta \tilde{\Delta}'_\alpha \approx 0, \quad (6.24)$$

where  $\delta \tilde{\Delta}'_\alpha$  is the variation of  $\tilde{\Delta}'_\alpha = \frac{1}{\alpha-1} \ln [\text{Tr}(A^{1/2\alpha} \rho_N A^{1/2\alpha})^\alpha / \text{Tr}(\rho_N^\alpha)] - \beta(U_{N\alpha} - U_{T\alpha})$ . In this case it can be shown that  $\delta \tilde{\Delta}'_\alpha \approx 0$ . From Eq. (6.24), to the first order, we have

$$-\delta S_\alpha + \beta \delta U_{N\alpha} \approx 0. \quad (6.25)$$

Similarly, even if the states  $\rho_N + \delta\rho$ ,  $\rho_N$  and  $\rho_T$  are not mutually commuting, it can easily be shown that for the integer  $\alpha$ , the Sandwiched and traditional Rényi relative entropies vanish independently to first order. In this case, if the Clausius inequality is to be satisfied, it amounts to requiring that  $\delta\tilde{\Delta}'_\alpha \geq 0$  to first order in variation. Further, we consider an example of noncommuting states to supplement our observations.

Now, we explore the Clausius inequality for noncommuting  $\rho_{T\alpha}, \rho_N$  and  $\delta\rho$  in  $\alpha > 2$ . From Eq. (6.13), we get

$$\delta\tilde{S}_\alpha(\rho_N \parallel \rho_{T\alpha}) = -\delta S_\alpha(\rho_N) + \beta\delta U_{N\alpha} + \delta\tilde{\Delta}'_\alpha, \quad (6.26)$$

where  $\tilde{\Delta}'_\alpha = \frac{1}{\alpha-1} \ln [\text{Tr}(A^{1/2\alpha}\rho A^{1/2\alpha})^\alpha / \text{Tr}(\rho^\alpha)] - \beta(U_{N\alpha} - U_{T\alpha})$ . Using the data processing inequality for  $\alpha \in [\frac{1}{2}, \infty)$ , we have

$$-\delta S_\alpha(\rho_N) + \beta\delta U_{N\alpha} + \delta\tilde{\Delta}'_\alpha \leq 0. \quad (6.27)$$

Therefore, if  $\delta\tilde{\Delta}'_\alpha$  is either positive or vanishing to the first order then Clausius inequality holds for  $\alpha \in [\frac{1}{2}, \infty)$ . For integer  $\alpha$ , Eq. (6.27) becomes an equality, to the first order and hence, if the Clausius inequality is satisfied then  $\delta\tilde{\Delta}'_\alpha \geq 0$  to the first order. We show that  $\delta\tilde{\Delta}'_\alpha = 0$  to the first order, with an explicit example. All these results indicate that for the Clausius inequality to hold in general, for any  $\alpha$  and for any state,  $\delta\tilde{\Delta}'_\alpha$  has to be either positive or zero to the first order in the variation. We perform a numerical study to investigate the Clausius inequality for  $\alpha \geq 0$ . We also consider an analytical example for further investigations.

### Numerical study:

To explore Clausius inequality numerically, we consider, without loss of generality, the Hamiltonian of a qubit system to be  $H = E_1 |1\rangle\langle 1|$ . The thermal state of the system is given by  $\rho_{T\alpha} = p_0 |0\rangle\langle 0| + (1 - p_0) |1\rangle\langle 1|$  which fixes the inverse temperature as  $\beta = (p_0^\alpha + p_1^\alpha)(p_0^{1-\alpha} - p_1^{1-\alpha})/E_1(1 - \alpha)$ . The nonequilibrium state is taken as  $\rho_N = (p_0 + \delta q) |0\rangle\langle 0| + ((1 - p_0) - \delta q) |1\rangle\langle 1| + \delta q |0\rangle\langle 1| + \delta q |1\rangle\langle 0|$ . The variation of  $\rho_N$  is done by the Rényi thermal state preserving map  $\Upsilon$  such that  $\rho_N \xrightarrow{\Upsilon} \rho_N + \delta\rho = (p_0 + \delta q)\tau + (p_1 - \delta q)\eta$ , where  $\eta$  is an arbitrary state and  $\tau = (\rho_{T\alpha} - p_1\eta)/p_0$  [269]. Fig. 6.2, indeed indicates that the Clausius inequality is respected, in general, for all ranges of  $\alpha$ .

### Analytical example:

Without loss of generality, the Hamiltonian of the system can be considered as

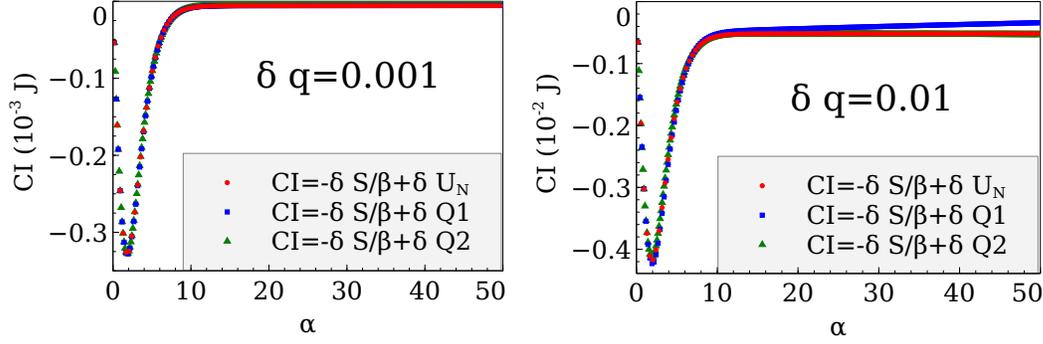


Figure 6.2: Clausius inequality for noncommuting quantum states for various values of  $\alpha$ : Along  $y$ -axis three different expressions for the Clausius inequality, which are the same to the first order, are plotted. The  $x$  axis is dimensionless and  $y$  axis has the dimension of energy (Joule). Here,  $\delta Q_1 = \text{Tr}[d\rho_N^\alpha(H - U_{N\alpha})]/\text{Tr}\rho_N^\alpha$  and  $\delta Q_2 = \text{Tr}[d\rho_N^\alpha(H - U_{T\alpha})]/\text{Tr}\rho_N^\alpha$ . We take  $E_1 = 1\text{J}$ ,  $p_0 = 0.7$  and  $\eta = 0.4|0\rangle\langle 0| + 0.6|1\rangle\langle 1| + 0.2|0\rangle\langle 1| + 0.2|1\rangle\langle 0|$ . The different plots are for two different values of  $\delta q$ .

$H = E_1|1\rangle\langle 1|$  [286]. Let the thermal state be given by

$$\rho_T = \begin{pmatrix} p_0 & 0 \\ 0 & p_1 \end{pmatrix}, \quad (6.28)$$

with  $p_0 + p_1 = 1$ . This fixes the inverse temperature as

$$\beta = \frac{p_0^\alpha + p_1^\alpha}{E_1(1 - \alpha)}(p_0^{1-\alpha} - p_1^{1-\alpha}). \quad (6.29)$$

Consider a nonequilibrium state, which is close to the thermal state, as

$$\rho_N = (p_0 + 2\delta q)|e_0\rangle\langle e_0| + (p_1 - 2\delta q)|e_1\rangle\langle e_1|, \quad (6.30)$$

where  $|e_0\rangle = \frac{1}{\sqrt{1+2\delta q}}(1 + \delta q, \delta q)^T$  and  $|e_1\rangle = \frac{1}{\sqrt{1+2\delta q}}(-\delta q, 1 + \delta q)^T$ . Also, consider a small variation of  $\rho_N$ , given by

$$\rho_N + \delta\rho = (p_0 + \delta q)|e_0\rangle\langle e_0| + (p_1 - \delta q)|e_1\rangle\langle e_1|, \quad (6.31)$$

where  $\delta\rho = -\delta q|e_0\rangle\langle e_0| + \delta q|e_1\rangle\langle e_1|$ . Note that  $\rho_T$  does not commute with  $\rho_N$  and  $\rho_N + \delta\rho$ . For this example, we have shown that the Clausius inequality is satisfied as an equality to the first order in  $\delta q$  and furthermore, it is shown that  $\delta\tilde{\Delta}'_\alpha$  is indeed zero.

As a consequence of the variation  $\rho_N \rightarrow \rho_N + \delta\rho$ , the change in the entropy of

the system is given by

$$\begin{aligned}
-\delta S_\alpha &= -[S_\alpha(\rho_N + \delta\rho) - S_\alpha(\rho_N)] \\
&= -\frac{1}{1-\alpha} [\ln\{\text{Tr}[(\rho_N + \delta\rho)^\alpha]\} - \ln\{\text{Tr}[\rho_N^\alpha]\}] \\
&= -\frac{1}{1-\alpha} [\ln\{(p_0 + \delta q)^\alpha + (p_1 - \delta q)^\alpha\} \\
&\quad - \ln\{(p_0 + 2\delta q)^\alpha + (p_1 - 2\delta q)^\alpha\}] \\
&= \frac{\alpha \delta q}{1-\alpha} \left[ \frac{p_0^{\alpha-1} - p_1^{\alpha-1}}{p_0^\alpha + p_1^\alpha} \right]. \tag{6.32}
\end{aligned}$$

Since the nonequilibrium state is close to the thermal state, the change in the internal energy is same as change in heat to the first order in variation, i.e.  $\delta Q_\alpha \approx U_{N\alpha}(\rho_N + \delta\rho) - U_{N\alpha}(\rho_N)$ , therefore, we have

$$\begin{aligned}
\delta Q_\alpha &\approx \frac{\text{Tr}[(\rho_N + \delta\rho)^\alpha H]}{\text{Tr}[(\rho_N + \delta\rho)^\alpha]} - \frac{\text{Tr}[\rho_N^\alpha H]}{\text{Tr}[\rho_N^\alpha]} \\
&= E_1 \frac{(p_0 + \delta q)^\alpha |\langle e_0 | 1 \rangle|^2 + (p_1 - \delta q)^\alpha |\langle e_1 | 1 \rangle|^2}{(p_0 + \delta q)^\alpha + (p_1 - \delta q)^\alpha} \\
&\quad - E_1 \frac{(p_0 + 2\delta q)^\alpha |\langle e_0 | 1 \rangle|^2 + (p_1 - 2\delta q)^\alpha |\langle e_1 | 1 \rangle|^2}{(p_0 + 2\delta q)^\alpha + (p_1 - 2\delta q)^\alpha} \\
&= \alpha \delta q E_1 \frac{p_1^\alpha (p_0^{\alpha-1} - p_1^{\alpha-1}) + p_1^{\alpha-1} (p_0^\alpha + p_1^\alpha)}{(p_0^\alpha + p_1^\alpha)^2} \\
&= \alpha \delta q E_1 \frac{(p_0 p_1)^{\alpha-1}}{(p_0^\alpha + p_1^\alpha)^2}. \tag{6.33}
\end{aligned}$$

Now, using Eq. (6.29), we have

$$\begin{aligned}
\beta \delta Q_\alpha &= \frac{\alpha \delta q}{1-\alpha} (p_0^{1-\alpha} - p_1^{1-\alpha}) \frac{(p_0 p_1)^{\alpha-1}}{(p_0^\alpha + p_1^\alpha)} \\
&= -\frac{\alpha \delta q}{1-\alpha} \left[ \frac{p_0^{\alpha-1} - p_1^{\alpha-1}}{p_0^\alpha + p_1^\alpha} \right]. \tag{6.34}
\end{aligned}$$

Combining Eq. (6.32) and Eq. (6.33), we get  $-\delta S_\alpha + \beta \delta Q_\alpha = 0$ . Therefore, the Clausius inequality is satisfied for all values of  $\alpha$ , for the qubit case considered above. Moreover, for this case, the variation in the sandwiched Rényi relative entropy can be shown to be zero to first order. The change in sandwiched Rényi relative entropy is given by

$$(1-\alpha) \delta \tilde{S}_\alpha(\rho_N || \rho_T) = \ln \text{Tr}[(A+B)^\alpha] - \ln \text{Tr}[A^\alpha], \tag{6.35}$$

where

$$A = \rho_T^{\frac{1-\alpha}{2\alpha}} (\rho_N + \delta\rho) \rho_T^{\frac{1-\alpha}{2\alpha}} = \sum_{i,j} a_{ij} |i\rangle \langle j|; \quad (6.36)$$

$$B = \rho_T^{\frac{1-\alpha}{2\alpha}} (-\delta\rho) \rho_T^{\frac{1-\alpha}{2\alpha}} = \delta q \sum_{i,j} b_{ij} |i\rangle \langle j|, \quad (6.37)$$

with  $a_{ij} = (p_i p_j)^{\frac{1-\alpha}{2\alpha}} \sum_k q_k \langle i | e_k \rangle \langle e_k | j \rangle$ ,  $q_0 = p_0 + \delta q$  and  $q_1 = p_1 - \delta q$  and  $b_{ij} = (p_i p_j)^{\frac{1-\alpha}{2\alpha}} \langle i | (|e_0\rangle \langle e_0| - |e_1\rangle \langle e_1|) | j \rangle$ . To the first order, we have  $a_{00} = p_0^{\frac{1-\alpha}{\alpha}} (p_0 + \delta q)$ ,  $a_{11} = p_1^{\frac{1-\alpha}{\alpha}} (p_1 - \delta q)$ ,  $a_{01} = (p_0 p_1)^{\frac{1-\alpha}{2\alpha}} \delta q (p_0 - p_1 + 2\delta q) = a_{10}$ ,  $b_{00} = p_0^{\frac{1-\alpha}{\alpha}}$ ,  $b_{11} = -p_1^{\frac{1-\alpha}{\alpha}}$ ,  $b_{01} = 0 = b_{10}$ . The eigenvalues of  $A$  are given by

$$\begin{aligned} \mu(s) &= \frac{a_{00} + a_{11} + s \sqrt{(a_{00} - a_{11})^2 + 4|a_{01}|^2}}{2} \\ &\approx \frac{a_{00} + a_{11} + s |a_{00} - a_{11}|}{2}, \end{aligned} \quad (6.38)$$

where  $s = \{1, -1\}$ . Similarly, the eigenvalues of  $(A + B)$  are given by

$$\nu(s) = \frac{c_{00} + c_{11} + s \sqrt{(c_{00} - c_{11})^2 + 4|c_{01}|^2}}{2}; \quad \{s = 1, -1\}, \quad (6.39)$$

where  $c_{ij} = a_{ij} + \delta q b_{ij}$ . To the first order, we have

$$\begin{aligned} &\sqrt{(c_{00} - c_{11})^2 + 4|c_{01}|^2} \\ &\approx |a_{00} - a_{11}| + \delta q \frac{(a_{00} - a_{11})(b_{00} - b_{11})}{|a_{00} - a_{11}|}. \end{aligned} \quad (6.40)$$

Therefore,  $\nu(s) = \mu(s) + \delta q m(s)$ , where  $\mu(s)$  is given by Eq. (6.38) and

$$m(s) = \frac{b_{00} + b_{11} + s \frac{(a_{00} - a_{11})(b_{00} - b_{11})}{|a_{00} - a_{11}|}}{2}. \quad (6.41)$$

For  $a_{00} \geq a_{11}$ , we have  $\mu(1) = a_{00}$ ,  $\mu(-1) = a_{11}$ ,  $m(1) = b_{00}$ ,  $m(-1) = b_{11}$ . For  $a_{00} \leq a_{11}$ , we have  $\mu(1) = a_{11}$ ,  $\mu(-1) = a_{00}$ ,  $m(1) = b_{11}$ ,  $m(-1) = b_{00}$ . Now,

$$\begin{aligned} \ln \text{Tr}[(A + B)^\alpha] &= \ln \sum_{s=\{-1,1\}} \mu(s)^\alpha + \alpha \delta q_0 \mu(s)^{\alpha-1} m(s) \\ &= \ln[\mu(1)^\alpha + \mu(-1)^\alpha] + \alpha \delta q \frac{\mu(1)^{\alpha-1} m(1) + \mu(-1)^{\alpha-1} m(-1)}{[\mu(1)^\alpha + \mu(-1)^\alpha]}. \end{aligned}$$

Also, we have  $\ln \text{Tr}[A^\alpha] = \ln[\mu(1)^\alpha + \mu(-1)^\alpha]$ . Therefore,

$$\begin{aligned}
(1 - \alpha)\delta\tilde{S}_\alpha(\rho_N||\rho_T) &= \alpha \delta q \left( \frac{\mu(1)^{\alpha-1}m(1) + \mu(-1)^{\alpha-1}m(-1)}{\mu(1)^\alpha + \mu(-1)^\alpha} \right) \\
&\approx \alpha \delta q_0 \left( \frac{a_{00}^{\alpha-1}b_{00} + a_{11}^{\alpha-1}b_{11}}{a_{00}^\alpha + a_{11}^\alpha} \right) \\
&\approx \alpha \delta q_0 \left( \frac{p_0^{\frac{\alpha-1}{\alpha}} p_0^{\frac{1-\alpha}{\alpha}} - p_1^{\frac{\alpha-1}{\alpha}} p_1^{\frac{1-\alpha}{\alpha}}}{p_0 + p_1} \right) \\
&\approx 0, \tag{6.42}
\end{aligned}$$

where in the second line we have used values of  $\mu(s)$  and  $m(s)$  for the case  $a_{00} \geq a_{11}$ . It can be seen easily that the second line is the same for the case  $a_{00} \leq a_{11}$ , too. Therefore,  $\delta\tilde{S}_\alpha(\rho_N||\rho_T) \approx 0$ . Hence, for this case, we have  $\delta\tilde{\Delta}'_\alpha$  vanishing to first order, thereby supporting our observation.

Thus, we have the following results: the Clausius inequality holds (i) for  $\alpha \in [0, 2]$  which follows from the data processing inequality for the traditional Rényi case, and (ii) for  $\alpha \in [\frac{1}{2}, \infty)$  provided  $\delta\tilde{\Delta}'_\alpha$  is either positive or vanishing to the first order, which follows from the data processing inequality for the Sandwiched Rényi case. Moreover, the difference in the data processing inequalities [194, 209, 210, 284] for the two relative entropies is yet another manifestation of the different quantum features of the two, which is captured nicely in the context of Clausius inequality.

## 6.7 Chapter summary

To formulate a complete theory of quantum thermodynamics based on the Rényi formalism, we explicitly derive the generalized first law of thermodynamics, starting from the Rényi thermal state. The Rényi thermal state basically defines equilibrium temperature and hence the zeroth law of thermodynamics. The main thrust of this chapter is to point out that the second laws of thermodynamics can be consistently derived based on the Rényi entropy and its relative versions. The overarching principle here is the well-known MaxEnt principle, given internal energy constraint.

Beyond equilibrium, the notion of heat and work is not so well defined and whether the second law of thermodynamics is valid in this regime is an intriguing question. We have successfully demonstrated that the proper identification of heat and work beyond equilibrium, in fact, plays the pivotal role to establish a valid second law which is respected universally. To correctly identify heat and work be-

yond equilibrium that is consistent with the second law of thermodynamics, we have exploited the equilibrium entropy associated with thermal density matrix and the relative entropy between an arbitrary density matrix and the thermal density matrix. Further, we have established that the *universality* of the second law of thermodynamics based on the Carnot statement is the manifestation of this form invariance of free energy which holds even beyond equilibrium.

Using the data processing inequalities for the traditional and the sandwiched relative Rényi entropies we establish the validity of the Clausius inequality and hence strengthen the second laws of thermodynamics developed here. Our results, specifically, the monotonicity of free energy pave the way to an operational resource theory of quantum thermodynamics with the Rényi thermal state being the free state and the allowed operations being the Rényi thermal state preserving maps. In this way, we have exhibited another important connection between the concepts of information theory and thermodynamics in modern quantum framework. It may not be out of place here to point out the changes that the Rényi thermal state entails two known frameworks based on the Gibbs thermal state: (a) the Green function theory of many-particle systems [287, 288, 289] and hence also (b) the Kubo-Martin-Schwinger (KMS) condition [289].

**N.B.** This chapter is mainly based on original work. We have started from the Rényi thermal state derived using MaxEnt principle in [274] and establish the first law of quantum thermodynamics in the Rényi entropic formulation. In establishing the first and second laws of quantum thermodynamics, we have correctly identified accessible work and heat exchange both in equilibrium and non-equilibrium cases. The free energy (internal energy minus temperature times entropy) remains unaltered, when all the entities entering this relation are suitably defined. Using Rényi relative entropies we have shown that this form invariance holds even beyond equilibrium and has profound operational significance in isothermal process. These results reduce to the Gibbs-von Neumann results when the Rényi entropic parameter approaches 1. We show that the universality of the Carnot statement of the second law is a consequence of the form invariance of the free energy, which is in turn the consequence of maximum entropy principle. Further, the Clausius inequality, which is the precursor to the Carnot statement, is also shown to hold based on the data processing inequalities for the traditional and sandwiched Rényi relative entropies. Thus, we find that the thermodynamics of nonequilibrium state and its deviation from equilibrium together determine the thermodynamic laws.

The result of this chapter has been published in “*Quantum Rényi relative entropies affirm universality of thermodynamics*, A. Misra, U. Singh, M. N. Bera, A.K. Rajagopal, *Phys. Rev. E*, **92**, 042161 (2015).”



## Summary and future directions

Thermodynamics has always been experimentally motivated. Its purpose is to develop principles that tell us what types of machines we can build, and what are the limits of their performance. Our ability to manipulate a physical system depends on the information about the system. Therefore, recent study to understand the thermodynamics of quantum systems have been inspired by quantum information theory to a great extent. In this thesis, we have investigated some important thermodynamic aspects of quantum coherence and correlations. The present thesis encompasses the interplay between the resource theory of quantum coherence and thermodynamics, role of generalized quantum correlations in detecting quantum phase transitions in the laboratory, importance of maximum entropy principle to establish the universality of the Carnot limit in quantum thermodynamics. The main points of the thesis and possible future directions inspired by the analysis of the work carried out in this thesis are highlighted as follows:

- How much work can be extracted from quantum states harnessing its quantumness has been of prime interest recently. The extraction of work from quantum states has been the subject of many fruitful investigations. This has led to useful insights into the role of coherence, correlations, and entanglement for work extraction. In turn it is also important to look into the work cost for establishing correlations and coherence. We have explored the intimate connections between the resource theory of quantum coherence and thermodynamic limitations on the processing of quantum coherence. In particular, we have studied the creation of quantum coherence by unitary transformations with limited energy. We go on even further to present a comparative investigation of creation of quantum coherence and mutual information within the

imposed thermodynamic constraints. We have found the maximal coherence that can be created under unitary operations starting from a thermal state and the unitary transformation that creates the maximal coherence. We have also found the maximal achievable coherence under the constraint on the available energy. We have established that when maximal coherence is created with limited energy, the total correlation created in the process is upper bounded by the maximal coherence and vice versa. For two qubit systems we have shown that there does not exist any unitary transformation that creates maximal coherence and maximal total correlation simultaneously with a limited energy cost. It would be interesting to explore what happens for quantum states with arbitrary number of parties and arbitrary dimensions. Our results are relevant for the quantum information processing in physical systems where thermodynamic considerations cannot be ignored. Thermodynamic protocols based on unitary operations will be an interesting aspects of future investigations. The recent developments in the resource theory of quantum thermodynamics are yet to meet the experimental tests. For example, the global entangling unitaries that can extract work from passive but not completely passive states are not realizable in the laboratory. This indicates the discrepancy between theoretically extractable work and the practical one. Optomechanical systems provide suitable testbeds for quantum thermodynamic concepts. Investigating these quantum thermodynamic issues in optomechanical setups and establishing the possibilities and impossibilities will be challenging. Investigating the energy cost of creating coherence and correlations in optomechanical systems is a potential domain for future exploration. Some pertinent questions to ask are: (i) How much work can be extracted maximally from a quantum states using unitary or any other restricted class of operations? (ii) What is the best initial state to extract work from? (iii) What will be the optimal strategies to store work in quantum states? (iv) What are the possibilities and impossibilities in the domain of Gaussian operations? These are some important questions which can be studied based on the optomechanical setups.

- We have introduced a class of quantum correlation measures as differences between total and classical correlations, in a shared quantum state, in terms of the sandwiched relative Rényi and Tsallis entropies. We have shown that the measures satisfy all the plausible axioms for quantum correlations. We have also demonstrated that the measures can faithfully detect the quantum critical point in the transverse quantum Ising model and find that they can be used

to remove an unquieting feature of nearest-neighbor quantum discord in this respect. Moreover, the measures provide better finite-size scaling exponents of the quantum critical point than the ones for other known order parameters, including entanglement and information-theoretic measures of quantum correlations. An obvious domain for future investigations is to examine the role of generalized quantum correlations to detect phase transitions in finite temperature scenarios. Another fruitful direction to explore is to study quantum phase transitions in other spin models such as symmetric  $XXZ$  model, Lipkin-Meshkov-Glick (LMG) model, anisotropic  $XY$  chain, etc. It has been shown in Ref. [290] that transverse field  $XY$  spin model, entanglement measures are always ergodic, while discord and work deficit are not for specific values of the transverse field. Whether generalized quantum correlations are ergodic or not in these aforesaid spin models are important questions to inquire. It would also be interesting to investigate whether the generalized quantum correlations are useful to detect topological phases of matter.

- Exploiting the generalized entropy we have established that the principle of maximum entropy affirms that no engine can be more efficient than the Carnot engine even harnessing quantum resources. To establish the universality of the Carnot statement of the second law of thermodynamics, we have formulated a complete theory of quantum thermodynamics in the Rényi entropic formalism exploiting the Rényi relative entropies, starting from the maximum entropy principle. In establishing the first and second laws of quantum thermodynamics, we have *correctly* identified accessible work and heat exchange both in equilibrium and non-equilibrium cases. The free energy (internal energy minus temperature times entropy) remains unaltered, when all the entities entering this relation are suitably defined. Exploiting Rényi relative entropies we have shown that this “form invariance” holds even beyond equilibrium and has profound operational significance in quantifying accessible work in isothermal process. These results reduce to the Gibbs-von Neumann results when the Rényi entropic parameter  $\alpha$  approaches 1. Moreover, it is shown that the *universality* of the Carnot statement of the second law is the consequence of the form invariance of the free energy, which is in turn the consequence of maximum entropy principle. Further, the Clausius inequality, which is the precursor to the Carnot statement, is also shown to hold based on the data processing inequalities for the traditional and sandwiched Rényi relative entropies. Thus, we have shown that the thermodynamics of nonequilibrium state and its de-

viation from equilibrium together determine the thermodynamic laws. This is another important manifestation of the concepts of information theory in thermodynamics when they are extended to the quantum realm. Our work is a substantial step towards formulating a complete theory of quantum thermodynamics and corresponding resource theory based on the generalized entropies. The Rényi entropy is essential to describe the physics and thermodynamics of fractals and multi-fractals systems. A full fledged resource theory based on the Rényi entropy would be fruitful to study the thermodynamics of fractals and multi-fractals systems.

Considering the ever increasing interest of quantum thermal machines, apart from surpassing the classical performance bounds, the ultimate performance limits, efficiency at maximum power, possibility of breaking Nernst's third law of these thermal machines will be interesting fields of investigation. How the presence of quantum coherence or correlations can enhance the performance of quantum thermal machines is an important query which still lacks reasonable understanding. The operation of a heat engine based on a driven three-level working fluid is shown to be better in the presence of coherence of the working fluid [42]. However, on the contrary it has been pointed out that quantum coherence may be detrimental to the speed of a minimal heat engine model based on a periodically modulated qubit [118], hybrid (of continuous and reciprocating) cycle heat engine [119]. This clearly tells us that quantum coherence is at best optional. Therefore, further study is needed to resolve these issues. Identifying the quantum thermodynamics signatures in thermal machines still remains elusive. Quantum absorption refrigerator (QAR) can be a ideal testbed to examine quantum thermodynamic signatures. Recently, we have shown QAR in the transient regime provides better cooling in terms of the speed and efficiency. Moreover, the transient regime can be exploited to examine the quantum thermodynamic signatures before the detrimental effects of the Markovian baths kick in. Studying the quantum thermal machines in presence of non-Markovian baths would be interesting. How the partial reversibility of work and entropy achieved in these non-Markovian domain can be exploited to enhance the performances of quantum thermal machines is an interesting problem. The spin bath models provide a platform to study the quantum thermal machines in the non-Markovian and strong coupling regime which can have far reaching impact. Proper identification of heat and accessible work is crucial in analyzing performance of quantum thermal machines. When

we venture on the less explored nonadiabatic, strongly coupled, non-Markovian domains we must ensure that proper identification of heat and work has been done which is operationally well motivated and consistent with the physical principles. Only then one can test whether quantum thermal machines can outperform their classical counterparts. We aim to revisit these fundamental issues in a systematic manner for quantum thermal machines in future.



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