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Gauge invariant quantum thermodynamics: Foundations and applications to critical systems

Termodinâmica quântica invariante de calibre: Fundamentos e aplicações em sistemas críticos

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GABRIEL FERNANDEZ FERRARI MELO

Gauge invariant quantum thermodynamics: Foundations and applications to critical systems

Termodinâmica quântica invariante de calibre: Fundamentos e aplicações em sistemas críticos

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1. Termodinâmica quântica. 2. Grupo termodinâmico. 3. Calor em sistemas fechados. 4. Coerências quânticas. 5. Simetrias. I. Céleri, Lucas Chibebe, orient. II. Título.

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UNIVERSIDADE FEDERAL DE GOIÁS

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ATA DE DEFESA DE DISSERTAÇÃO

Ata nº 226 da sessão de Defesa de Dissertação de Gabriel Fernandez Ferrari Melo, que confere o título de Mestre em Física, na área de concentração em Física.

Aos 04 dias do mês de abril de 2025, a partir das 09h00min, por meio de videoconferência, realizou-se a sessão pública de Defesa de Dissertação intitulada "Gauge invariant quantum thermodynamics: Foundations and applications to critical systems". Os trabalhos foram instalados pelo Orientador, Professor Doutor Lucas Chibebe Céleri (IF/UFG), com a participação dos demais membros da Banca Examinadora: Professor Doutor Thiago Rodrigues de Oliveira (IF/UFF), membro titular externo; e Professor Doutor Norton Gomes de Almeida (IF/UFG), membro titular interno. Durante a arguição, os membros da banca não fizeram sugestão de alteração do título do trabalho. A Banca Examinadora reuniu-se em sessão secreta a fim de concluir o julgamento da Dissertação, tendo sido o candidato aprovado pelos seus membros. Proclamados os resultados pelo Professor Doutor Lucas Chibebe Céleri, Presidente da Banca Examinadora, foram encerrados os trabalhos e, para constar, lavrou-se a presente ata que é assinada pelos membros da Banca Examinadora, aos 04 dias do mês de abril de 2025.

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“If physical theories were people, thermodynamics would be the village witch. Over the course of three centuries, she smiled quietly as other theories rose and withered, surviving major revolutions in physics, like the advent of general relativity and quantum mechanics. The other theories find her somewhat odd, somehow different in nature from the rest, yet everyone comes to her for advice, and no-one dares to contradict her. ”

J. Goold, M.Huber, A.Riera, L.del Rio and Psryzpezyk [1].

“A todos que já duvidaram de si mesmos em sua jornada acadêmica: acreditem, somos capazes!”

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List of Publications

The original results presented in this dissertation have been previously reported in collaboration with Lucas C. Céleri and Łukasz Rudnicki in the following paper,

Quantum thermodynamics as a gauge theory,
G. F. Ferrari, L. Rudnicki, and L. C. Céleri
Accepted for publication in Phys. Rev. A (2025),
Preprint available at: arXiv:2409.07676 [2].

Resumo

Neste trabalho, formalizamos e estendemos o approach para a termodinâmica quântica como uma teoria de gauge, inicialmente proposta por Céleri e Rudnicki na Ref. [3]. Nesse formalismo, as quantidades termodinâmicas são descritas como funcionais do operador densidade e emergem de um processo de *Coarse-graining* sobre todas as transformações unitárias que preservam a energia do sistema - conjunto que denominamos grupo termodinâmico. Essa abordagem incorpora intrinsicamente as limitações de acesso informacional ao sistema, restrito ao conhecimento de medições na base de energia. Nossa contribuição generaliza as expressões para calor e trabalho invariantes além do tratamento apresentado em [3], incluindo explicitamente a consideração de níveis de energia degenerados dinâmicos. Mais que uma extensão formal, estabelecemos uma interpretação física rigorosa dessas quantidades através da dinâmica não unitária do estado efetivo obtido pelo *Coarse-graining* induzido pelo grupo termodinâmico. Demonstramos que a restrição fundamental a medições na base de energia implica na inacessibilidade de parte da energia do sistema, interpretada como um calor efetivo associado à produção de coerências na base de energia. Consequentemente, o trabalho derivado corresponde ao trabalho efetivo do sistema, com sua contribuição energética reduzida pela parcela alocada como calor. No contexto da segunda lei, introduzimos a entropia invariante de gauge, provando que satisfaz todas as propriedades requeridas para uma entropia termodinâmica. Essa entropia apresenta uma dependência explícita do grupo termodinâmico, manifesta através de uma contribuição entrópica diretamente vinculada às degenerescências do espectro do Hamiltoniano. Crucialmente, identificamos que a origem da produção de entropia coincide com a do calor em sistemas fechados, ambas emergindo da não-unitariedade inerente à dinâmica do estado de *Coarse-graining*. Como aplicação final, implementamos nosso formalismo na dinâmica quântica de sistemas de spins sujeitos a *quenches*, revelando que o calor coerente captura assinaturas de irreversibilidade. Em sistemas críticos, as quantidades derivadas nesta teoria provam-se fundamentais para entender as modificações na estrutura de simetrias do sistema em relação às simetrias internas do grupo de gauge termodinâmico.

Palavras-chave: Termodinâmica quântica; Grupo termodinâmico; Calor em sistemas fechados; Coerências quânticas; Simetrias.

Abstract

In this formalism, thermodynamic quantities are described as functionals of the density operator and emerge from a coarse-graining process over all unitary transformations that preserve the system's energy - a set we refer to as the thermodynamic group. This approach intrinsically incorporates informational access limitations to the system, constrained to energy basis measurements. Our contribution generalizes the expressions for invariant heat and work beyond the treatment presented in [3], explicitly including the consideration of dynamic degenerate energy levels. More than a formal extension, we establish a rigorous physical interpretation of these quantities through the non-unitary dynamics of the effective state obtained by the coarse-graining induced by the thermodynamic group. We demonstrate that the fundamental restriction to energy basis measurements implies the inaccessibility of part of the system's energy, interpreted as an effective heat associated with the production of coherences in the energy basis. Consequently, the derived work corresponds to the system's effective work, with its energetic contribution reduced by the portion allocated as heat. Within the second law context, we introduce the gauge-invariant entropy, proving it satisfies all required properties for a thermodynamic entropy. This entropy exhibits an explicit dependence on the thermodynamic group, manifested through an entropic contribution directly linked to the Hamiltonian's spectral degeneracies. Crucially, we identify that the origin of entropy production coincides with that of heat in closed systems, both emerging from the inherent non-unitarity in the coarse-grained state's dynamics. As a final application, we implement our formalism in the quantum dynamics of spin systems undergoing quenches, revealing that coherent heat captures signatures of irreversibility. In critical systems, the quantities derived within this theory prove fundamental for understanding modifications in the system's symmetry structure relative to the internal symmetries of the thermodynamic gauge group.

Keywords: Quantum thermodynamics; Thermodynamic group; Heat in closed systems; Quantum coherences; Symmetries.

Contents

List of Figures

Chapter 1

Introduction

Among the physical theories, thermodynamics certainly stands out as an extremely peculiar theory. Indeed, fundamental theories such as General Relativity and the Standard Model of particle physics aim to describe how processes and interactions occur in their respective regimes. However, thermodynamics is constructed from a different perspective, which instead of progressing in the same direction, focuses on establishing the conditions and limitations for which physical processes can occur and, most importantly, which processes cannot occur in nature.

This distinctive character of thermodynamics is, in essence, what differentiates it from other physical theories. Moreover, this type of description possesses a certain operational character which guides thermodynamics to a certain universality intrinsic to the theory. In fact, these subtleties of the theory have led various physicists to understand and recognize thermodynamics as a solid pillar within Physics, which probably should not be violated[4]. Particularly, in Ref.[1], the authors present a simple passage that, in a poetic way, encapsulates the strength and universality of thermodynamics, which we quote below.

> If physical theories were people, thermodynamics would be the village witch. Over the course of three centuries, she smiled quietly as other theories rose and withered, surviving major revolutions in physics, like the advent of general relativity and quantum mechanics. The other theories find her somewhat odd, somehow different in nature from the rest, yet everyone comes to her for advice, and no-one dares to contradict her. [1]

In this passage, the "witch of physical theories" is exalted not only for its generality and extent of validity but also for its unwavering persistence throughout the development of other physical theories. Certainly, referring to thermodynamics as a "witch" is extremely interesting in the context of comparing it to other physical theories. However, the last sentence of this passage suggests that labeling thermodynamics as just any "witch" might not be very fitting; perhaps elevating it to the title of "oracle[1]" of physical theories places it in the position that thermodynamics truly deserves.

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[1] Oracles were priests or priestesses residing in sacred places in ancient Greece, consulted by people to receive answers and guidance from the gods on personal and political matters.

In the classical context, the wisdom of this "oracle" is essentially founded on the existence of three laws. Indeed, the zeroth law of thermodynamics establishes the conditions for thermodynamic systems to be in states of equilibrium, which are, in summary, the states in which thermodynamic description is made. The first law of thermodynamics moves in the direction of a generalization of the principle of conservation of mechanical energy, which can be summarized as the energy of the universe being constant [4]. Finally, the second law of thermodynamics guides us to an understanding of which physical processes can occur, thus establishing conditions of validity and limits for their realization. From a quantum perspective, it is still possible to consider a third law, which ensures a relationship between the entropy established by the second law and the thermodynamic temperature, asserting that the entropy of a system is zero at absolute zero temperature [5].

The laws of thermodynamics are the fundamental tools that ensure its universality, which essentially lies in the type of questions thermodynamics aims to resolve. In effect, all of classical thermodynamics is constructed on the notion that measurements, in the thermodynamic limit, are, in essence, a coarse-graining of space and time intervals. Through this coarse-graining, thermodynamic variables emerge from the averages of dynamic microscopic variables, which are not measured by any macroscopic apparatus. As a result, thermodynamics establishes itself as a robust theory that sets limits on physical processes since microscopic degrees of freedom are eliminated by coarse-graining. Consequently, this introduces an independence of the theory from the microscopic description of the system. Because of this, thermodynamics can then be applied to an extremely wide range of physical systems, such as in engineering, biology, neuroscience [6–8], as well as in complex systems [9], computing [10], and even in black holes [11].

However, when we consider equilibrium states, which are the states where classical thermodynamics is established, a certain characteristic becomes prominent. Indeed, in equilibrium states in the thermodynamic limit, the net flows of all quantities are zero, and consequently, microscopic fluctuations are negligible. In fact, within the thermodynamic limit, these fluctuations can be ignored, as the descriptions emerge as averages from spatial and temporal coarse-graining. Nevertheless, as we move into systems far from the thermodynamic limit, for example in very small systems, the usual formulation of thermodynamics ceases to be applicable. In such cases, it is necessary to employ other approaches for studying systems, particularly stochastic thermodynamics [12]. Additionally, other formulations of thermodynamics can also be considered, such as those based on information theory [1] and elegant axiomatic formulations [13, 14]. In these formulations, fluctuations previously ignored become amenable to consideration in systems described by states out of equilibrium.

Nonetheless, when we begin to delve into the realm of quantum systems, the laws of quantum mechanics become relevant. Thus, understanding how aspects of classical thermodynamics can be translated into the quantum context becomes significant. In this regard, the seminal work of Robert Alicki [15] plays a significant role in this description, as it introduces the notions of heat and work in the context of quantum thermal machines. However, a complete, robust, and fully consistent theory of quantum thermodynamics has not yet been fully developed [16, 17]. In this context, several questions remain open, particularly understanding how thermodynamic quantities such as work, heat, and entropy should be defined in the quantum scenario.

In particular, different approaches are being explored to define how these quantities should be established. For instance, work is generally defined as changes in the energy of the system due to external modifications resulting from some time-dependent process. Moreover, the Hamiltonian of the system must be modified through one or a family of Hamiltonian parameters.

Furthermore, a common method of evaluating work in this sense is the two-point measurement scheme, where work is defined as the difference in energy between two projective measurements of the Hamiltonian at the beginning and end of the process [18, 19]. This definition treats work as a stochastic variable and, in the context of quantum systems, work then gives way to average work, which is associated with the averages of individual quantum trajectories [20]. Nonetheless, other definitions may also be considered, such as those involving the coherence elements of the density operator [21].

Similarly to work, notions of heat and their definitions in the quantum context are also discussed. In his seminal work, Alicki [15] introduces the notion of heat as a physical quantity that emerges in open systems, that is, when the physical system is in contact with a reservoir, causing the evolution of the system to be non-unitary. Specifically, in this context, closed quantum systems should not present heat contributions due to any change in the Hamiltonian. However, there are works that provide definitions of heat even for closed quantum systems [22–24]. In this context, the notion of heat acquires additional meanings, which can sometimes be related to uncertainties in the energy basis [22–24].

Furthermore, another important issue in constructing quantum thermodynamics lies in defining thermodynamic entropy. Indeed, various schools of thought have emerged in this area, guided by different philosophical perspectives [25, 26]. The Von Neumann entropy [27], which is consistent with the Gibbs entropy for thermal states, does exist; however, it presents some inconsistencies as a thermodynamic entropy [26]. Nonetheless, other significant notions of entropy can also be elaborated, such as Boltzmann entropy, observational entropy, and diagonal entropy [25, 26]. In particular, diagonal entropy stands out due to its direct connection with the energy basis of the system, more precisely, with the diagonal elements of the density operator in the energy basis of the system's Hamiltonian [28].

Moreover, information theory itself provides a family of definitions for entropic quantities, with relative entropy being substantially important in the context of quantum thermodynamics. Relative entropy quantifies the "distance"[2] between two quantum states and is fundamental to

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[2] Strictly speaking, relative entropy is not a metric in the traditional sense of distance. However, this notion of entropy provides a measure of distinguishability between quantum states, justifying the use of the term "distance." Moreover, it is possible to construct a metric from relative entropies through simple symmetrization. In Appendix A.2, these aspects are discussed.

the concept of irreversibility and the arrow of time in quantum processes [29–31].

In light of these various open questions, a recent work proposed a new formulation for quantum thermodynamics as a gauge theory [3]. In this work, Céleri and Rudnicki, inspired by the success of fundamental theories, particularly field theories such as General Relativity and the Standard Model of particle physics, introduced the notion of a thermodynamic gauge group. The transformations of the thermodynamic group form the basis for constructing physical quantities that would be invariant under the action of this group. These physical quantities would then be obtained through a process of coarse-graining, similar to classical thermodynamics.

Thus, the theoretical framework introduced in Ref. [3] defines a symmetry structure known as the Thermodynamic Gauge Group, or thermodynamic group, which facilitates a type of coarse-graining within the informational realm. Just as the detailed microscopic dynamics of a classical system can be irrelevant to Thermodynamics, a portion of the information within a quantum state becomes superfluous for Quantum Thermodynamics. The thermodynamic group was specifically designed to eliminate this superfluous information. Hence, Quantum Thermodynamics is described as a gauge theory governed by this thermodynamic group. By invoking the principle of gauge invariance, quantum thermodynamic quantities are derived uniquely from this framework. Ref. [3] provides an extensive discussion on the gauge-invariant concepts of work and heat and their associations with quantum properties such as quantum coherences.

Moreover, an important issue concerning the establishment of the thermodynamic gauge group introduced in Ref. [3] arises. In essence, the thermodynamic gauge group is not fundamental, meaning it does not naturally originate from the mathematical underpinnings of the theory as seen in field theories. Instead, the thermodynamic gauge emerges from the coarse-graining paradigm, which is hypothesized by the theory. In analogy with conventional field theories, the density operator in this context becomes similar to potentials. As such, the density matrices, which act as the bearers of information, assume the role of these potentials. Consequently, the information within the system's state is deemed redundant exclusively from a thermodynamic viewpoint but retains its relevance in Quantum Information or Quantum Mechanics. Essentially, the thermodynamic group was devised to systematically eliminate such redundancy. Therefore, the function of the thermodynamic group is to transition from the state space to thermodynamic variables by excising redundant data, thus implementing a form of coarse-graining reminiscent of classical thermodynamics.

However, the initial developments proposed by Céleri and Rudnicki in Ref. [3] were still somewhat nascent. Indeed, this work addressed various issues within essentially specific contexts, necessitating broader generalization. Consequently, several aspects that were left unresolved include:

I) The consideration of Hamiltonian systems whose degeneracies do not change over time.

II) The understanding and interpretation of the obtained quantities—particularly heat in closed systems—still require further discussion.

III) The development following the first law, particularly the definition of an entropy obtained in an invariant manner, as well as a second law for the theory.

IV) Applications of the formalism to physical problems, particularly in many-body systems.

In this context, the present work emerges as a continuation, formalization, and generalization of the theory initially proposed by Céleri and Rudnicki in Ref. [3]. Our aim is essentially to address the four items mentioned above. For organizational purposes, as well as to summarize what will be done throughout the text, we will provide a brief description of the work below.

- Chapter 2 of this dissertation consists of a brief review of Thermodynamics. Indeed, in this chapter, we will present concepts and general notions regarding relevant physical quantities in the context of classical and quantum thermodynamics. Additionally, we will discuss some general aspects of certain definitions of entropy in the quantum context.

- In Chapter 3, we will construct the foundations of thermodynamics as a gauge theory. Thus, starting from a set of assumptions, we will build the thermodynamic group and subsequently establish the notion of physical quantities within this approach, which are invariant under the thermodynamic group. General aspects of the formalism will also be discussed.

- In Chapter 4, we will obtain the associated expressions for heat, work, and entropy within the formalism of the $\mathcal{G}_{\mathrm{T}}$-group. Then, we will revisit some of the basic applications developed by Céleri and Rudnicki in Ref. [3].

- In Chapter 5, we will obtain expressions for the heat and work, defined in an invariant manner, associated with out-of-equilibrium processes. We will also argue how these quantities connect with the notions of irreversibility and state asymmetry. Finally, we apply this approach to the study of two spin systems that exhibit quantum phase transitions, specifically:

    - The Landau-Zener model, which is solved analytically,
    - The Lipkin-Meshkov-Glick model, which we develop numerically,

  for both, we evaluate the main thermodynamic quantities (Heat, work, and entropy) throughout the quench process.

- In Chapter 6, we present a general discussion on the developments from the previous chapters and further explore some perspectives that have already been initially discussed and are left for future investigations.

In addition to the chapters presented, there are two appendices included at the end of the dissertation. In summary, these appendices were constructed with two main objectives. The first objective is related to the self-contained nature of the text, ensuring that it is comprehensive and accessible. To this end, we present some general results that span both the scope of quantum information theory and group theory, including Haar measures, which were employed throughout the text to derive the main results of each chapter. On the other hand, the second objective is rooted in the educational purpose of the dissertation. Specifically, the appendices were designed to provide potential readers with a brief introduction to the concepts and foundational elements that underpin the text, thereby serving as a didactic resource for readers who may not be as familiar with these topics.

Regarding the notations and constants, we will use a coordinate system where the constants $k_B = \hbar = 1$, with k_B being the Boltzmann constant and $\hbar$ the reduced Planck constant. In some cases, these constants may appear to clarify the topics discussed. However, we emphasize that all numerical and analytical calculations will treat these constants as 1.

Chapter 2

Thermodynamics: An overview

In this chapter, we will revisit some general aspects of classical and quantum thermodynamics. In short, the concepts and discussions presented here constitute part of some fundamental elements for the work that will be developed in the following chapters. Indeed, our goal here is to go through some particular elements of thermodynamics, especially the usual definitions of heat and work as well as the formulations of the first and second law.

2.1 Classical Thermodynamics

Thermodynamics, unlike most physical theories, does not concern itself with describing the mysteries of the natural world. However, it provides us with a robust formalism on how to explore this world, for example, by indicating suitable routes for extracting resources, such as hot gas or magnetized metal, to achieve specific objectives, whether moving a train or formatting a hard drive [1]. Moreover, thermodynamics also establishes the limitations for these explorations, imposing fundamental constraints on the processes of energy and matter transformation, delineating what is possible and what is unattainable [1].

In fact, the early developments of thermodynamics traverse an extensive historical journey of empirical results [32–38] which guide us to its modern axiomatic formulation [5]. In this context, the foundations of thermodynamics are laid out in a set of postulates that synthesize the results obtained throughout its development. Furthermore, the nature of macroscopic measurement processes is rigorously grounded in the Central Limit Theorem [39].

In particular, macroscopic measurements are established under the assumptions of being extremely slow compared to the atomic time scale and are extremely coarse on the atomic scale of distance. Indeed, these two assumptions about the macroscopic measurement process ensure not only simplicity in the description of these systems but also a universal character for thermodynamics.

This description is what we call coarse-graining, which, in this context, emerges from the impossibility of determining all the microscopic details of a macroscopic system. Consequently, we do not evaluate the individual components of the system, as microscopic fluctuations are expected to average out over time and space, thus forming a well-defined behavior for laws and average physical quantities that are independent of microscopic details.

In this sense, note that in a macroscopic measurement, the atoms composing the system undergo extremely rapid and complex movements. However, since macroscopic measurements are extremely slow on the atomic time scale, any sets of atoms associated with rapidly oscillating movements should, on average, cancel out over time and not contribute to the system's description. Nevertheless, a particular set of combinations of atomic coordinates, which are time-independent, will be macroscopically observable [5].

The surviving atomic coordinates are then those that have characteristic times similar to the measurement method employed. As a result, the hypothesis that macroscopic measurements are extremely slow on the atomic time scale reveals that thermodynamics describes only static macroscopic systems.

Furthermore, macroscopic measurements are also coarse on the atomic scale of distance. Indeed, the motion of individual atoms is strongly coupled; consequently, these atoms tend to organize and move in patterns called normal modes. That is, it becomes more convenient to describe an atomic state by specifying the instantaneous amplitudes of each normal mode. These amplitudes are called normal coordinates, and there are exactly the same number of normal coordinates as atomic coordinates [5].

Consequently, spatial averages over these macroscopic systems do not consider individual atoms but rather sets that can be identified in their measurement. As a result, it is the normal modes associated with long wavelengths that survive in spatial averages. Since these modes have a spatially homogeneous structure, they survive spatial averaging. Moreover, it is these same low-frequency normal modes that survive temporal averaging, as the contributions from high-frequency modes should cancel out on average [5].

Note that the surviving coordinates, which may be of different natures, form the set of thermodynamic variables. Indeed, the study of these surviving coordinates forms areas of physics such as Mechanics and Electricity. On the other hand, thermodynamics is concerned with the manifestations of effects from the numerous atomic coordinates that, due to the coarseness of macroscopic observations, do not explicitly appear in the macroscopic description of the system.

In this sense, there are two strictly important consequences for thermodynamics that result from these hidden modes. The first consequence is that these modes can be used as repositories and carriers of energy. For example, energy transferred by mechanical and electrical modes is respectively termed mechanical work and electrical work. Nevertheless, it is also possible that hidden modes of motion, associated with high frequencies, can be used to transfer energy within a system. In particular, the transfer of energy through these hidden modes is what we call heat [5].

This discussion synthesizes some notions about measurement processes, particularly in thermodynamics. In this sense, note that thermodynamics is a theory that essentially describes average quantities based on an elegant coarse-graining in macroscopic systems. Furthermore, note that the entire discussion does not make any assumptions about the nature of the thermodynamic coordinates, highlighting the universality of the theory.

2.1.1 Axiomatic formulation of thermodynamics

Once we have determined the scope of interest of thermodynamics, we will proceed to its construction. Indeed, classical thermodynamics can be set in an axiomatic formulation [5]. In this sense, the description of a closed system, i.e., one that can only interact with another system through a sufficiently controlled transfer of energy, is usually made in terms of the quantities: volume V, mole number of the k-th chemical component N_k, and internal energy U, and is based on three postulates. The first postulate is associated with the existence of equilibrium states, which we present below.

Postulate 1. *(Equilibrium [5]). There exist particular states (called equilibrium states) of simple systems that, macroscopically, are characterized completely by the internal energy* U*, the volume* V*, and the mole numbers* $N_1, N_2, \ldots, N_k$ *of the chemical components.*

Equilibrium states form a manifold of thermodynamic states in which there are no macroscopic changes over time. Indeed, Postulate 1 is equivalent to characterizing an equilibrium state as a thermodynamic state in which all net fluxes within the system cancel out. Moreover, any state in a closed system, in classical thermodynamics, tends toward the equilibrium state.

That is, in a scenario where some process is carried out, causing the system to depart from equilibrium, once the system is closed again, the resulting state tends to return to the thermodynamic equilibrium state. In this context, we can then define the heat flux, for any process, as the difference between the change in internal energy and the work done in that process.

In this sense, let us consider a quasi-static process, that is, a thermodynamic process sufficiently slow such that the system never departs from equilibrium throughout the process. Then, the infinitesimal heat flux for this process is defined by:

$$\delta Q = \mathrm{d}\,\mathrm{U} - \delta W \tag{2.1}$$

where δ denotes an inexact differential, W and Q are, respectively, the total work and total heat flux. The inexact differentials that appear in Eq. (2.1) are associated with the fact that both work and heat flux in a closed system depend on the process. However, starting from Eq. (2.1), we can write:

$$\Delta\,\mathrm{U} = Q + W \tag{2.2}$$

where $\Delta \mathrm{U} = \mathrm{U}_f - \mathrm{U}_i$ with f and i labeling the final and initial states, respectively. Eqs. (2.1) and (2.2) correspond to the first law of thermodynamics.

However, it is important to note that Eq. (2.1) does not imply that internal energy is the sum of energy contributions from work and heat flux. Certainly, this becomes clear through Eq. (2.2), which shows that the sum of these contributions equals the change in internal energy.

Nevertheless, note that both expressions reveal that the first law of thermodynamics is a conservation law. More specifically, it details an energy balance between contributions from work and heat flux. Moreover, although Q and W depend on the thermodynamic process, the change in internal energy is independent of any process. In short, this is a consequence of the fact that the state function U is a conservative field.

Besides the state function U, other functions can be used to represent a thermodynamic state [5]. In particular, the second postulate of thermodynamics introduces a new state function that depends on extensive parameters (which scale with the system), such as internal energy, volume, and number of particles. In this sense, we introduce the second postulate.

Postulate 2. *(Existence of entropy [5]) There exists a function (called the entropy S) of the extensive parameters of any composite system, defined for all equilibrium states and having the following property: The values assumed by the extensive parameters in the absence of an internal constraint are those that maximize the entropy over the manifold of constrained equilibrium states.*

Note that Postulate 2 not only establishes the existence of entropy but also asserts that this quantity must be maximized in the manifold of equilibrium states. However, this postulate does not uniquely determine, nor even from any set of transformations, the behavior and properties that entropy must satisfy. The following postulate specifies the characteristics of entropy.

Postulate 3. *(Entropy properties [5]) The entropy of composite systems is additive over their constituent subsystems. Furthermore, entropy is a continuous and differentiable function almost everywhere, and it is a monotonically increasing function of energy, i.e*

$$\frac{\partial S}{\partial U} > 0. \tag{2.3}$$

The first property of thermodynamic entropy, as stated in Postulate 3, can be expressed by the following equality.

$$S = \sum_i S_i, \tag{2.4}$$

in which the total entropy function of a system S is expressed as the sum of the entropies S_i of each i-th subsystem. The assumptions of continuity and differentiability almost everywhere are specially important. Indeed, in various natural scenarios, particularly in thermodynamic equilibrium, entropy is expected to be continuous and differentiable. However, there are particular cases where this property may be violated. For example, during first- and second-order phase transitions, the entropy and its derivative, respectively, exhibit a discontinuity at the critical point of the system. Nevertheless, except on a set of measure zero, it is reasonable to assume that entropy is a function of class C^{∞}.

From Postulate 3, we can then define the concept of thermodynamic temperature. Indeed, the thermodynamic temperature T of a system, in a state of equilibrium, is defined by:

$$T \equiv \frac{\partial U}{\partial S} \quad \therefore \quad T > 0. \tag{2.5}$$

Note that the inequality $T > 0$ is a consequence of the monotonicity of entropy with respect to internal energy as defined by Postulate 3 and expressed by Eq. (2.3). From the definition of thermodynamic temperature, it becomes possible to specifically address thermal equilibrium and thus formulate the so-called zero law of thermodynamics, which establishes a transitivity relationship between systems in equilibrium.

Observe that, as established by Postulate 3, the temperature defined by Eq. 2.5 is strictly positive, in particular, it is non-zero. In fact, within the context of classical thermodynamics, we do not expect to encounter any system with zero temperature. However, in some scenarios, such as in quantum systems, we can have zero temperature. The possibility of having $T = 0$ leads us to the following postulate.

Postulate 4. *The entropy S for any system vanishes in the state for which*

$$\frac{\partial U}{\partial S} = 0,$$

that is, at the zero of temperature.

Postulate 4 sometimes appears in the literature as the third law of thermodynamics or even as Nernst's Postulate [5]. In truth, this postulate is only fully explained with quantum mechanics. However, the bulk of thermodynamics does not require this postulate [5]. Thus, Postulates 1, 2, and 3 establish all the essential characteristics for the definition of thermodynamic entropy. We will then proceed to the formulation of the second law of thermodynamics.

Unlike the first law, the second law of thermodynamics does not consist of a conservation principle or even an energy balance. In fact, the implications of the second law have another level of sophistication since it imposes limits on the occurrence of physical processes. In particular, one of the results establishing the second law was given by Clausius, who states that it is impossible to carry out a process whose only effect is to extract heat from a source at temperature T_c to a source at temperature $T_h > T_c$.

Mathematically, Clausius's result can be expressed by the following inequality:

$$\oint_C \frac{\delta Q}{T} \leq 0 \tag{2.6}$$

where C denotes a path between two points A and B. Equality in expression (2.6) occurs if and only if the path C is reversible, that is, along the entire trajectory C the thermodynamic state of the system is always in equilibrium. However, from Clausius's result, we can obtain a formulation of the second law in terms of entropy.

Indeed, let $U \equiv U(S, X)$ be the thermodynamic state function, where X is a set of parameters X_k that can be associated with different normal coordinates due to the nature of the system. Thus, it is possible to expand U as:

$$\mathrm{d}\,U = \mathrm{d}\,S\frac{\partial U}{\partial S} + \sum_k \mathrm{d}\,X_k\frac{\partial U}{\partial X_k} = T\,\mathrm{d}\,S + \sum_k \mathrm{d}\,X_k\frac{\partial U}{\partial X_k} \tag{2.7}$$

in which we assume that the quantities involved may depend on a parameter t, which could be time. Thus, by inspecting Eq. (2.1), we can identify the following equality

$$T\,\mathrm{d}\,S = \mathrm{d}\,Q, \tag{2.8}$$

since the variables X_k must specify contributions as work. Thus, it is immediate from the equality (2.8) that:

$$T\,\mathrm{d}\,S = \delta Q \implies \Delta S = \oint_{C_r} \frac{\delta Q}{T} \tag{2.9}$$

in which the path C_r is associated with a reversible process and $\Delta S = S_B - S_A$, where A and B are labels associated with two equilibrium states. Now, consider a process described by the path $C = C_i \cup (-C_r)$ where C_i refers to an irreversible process. From this and Clausius' inequality (2.6) we obtain:

$$\begin{aligned} \oint_{C=C_i\cup(-C_r)} \frac{\delta Q}{T} \leq 0 \quad &\implies \quad \oint_{-C_r} \frac{\delta Q}{T} + \oint_{C_i} \frac{\delta Q}{T} \leq 0 \\ &\implies \quad -\Delta S + \oint_{C_i} \frac{\delta Q}{T} \leq 0 \\ &\implies \quad \Delta S \geq \oint_{C_i} \frac{\delta Q}{T}. \end{aligned} \tag{2.10}$$

As discussed previously, equality in Eq. (2.10) holds if and only if C_i is a path associated with a reversible process. The expression given by Ineq. (2.10) corresponds to the second law of thermodynamics in terms of entropy. In particular, for an isolated system $\delta Q = 0$ and thus it follows that entropy must always increase.

Now, note that we can describe the quantities involved above with respect to the time t associated with the process we are considering. Consequently, the change in entropy can be written as $\Delta S = S(t) - S(0)$ and the inexact differential of heat can be written as $\delta Q = \dot{Q}\delta t$, and thus

Ineq (2.10) gives us

$$\frac{\mathrm{d}\,S}{\mathrm{d}\,t} \geq \frac{\dot{Q}}{T} \tag{2.11}$$

note that we consider the temperature T constant throughout the entire process. This consideration stems from a basic assumption that the heat exchange occurs with systems that are infinitely large compared to our system.

Thus, according to Ineq. (2.11), there must exist a non-negative quantity, which we will denote by $\dot{\sigma}(t)$, such that:

$$\frac{\mathrm{d}\,S}{\mathrm{d}\,t} = \frac{\dot{Q}}{T} + \dot{\sigma}(t). \tag{2.12}$$

Indeed, the quantity $\sigma(t)$ represents the entropy production in the system. In summary, this development provides us with another inequality for the second law, which is:

$$\dot{\sigma}(t) \geq 0, \tag{2.13}$$

that is, the rate at which entropy is produced in a system is always positive. Note that, in isolated systems, the notion of entropy production becomes equivalent to the temporal variation of entropy.

Notice that Eq. (2.12) shows that the second law is not some kind of conservation law since it is possible to see that the term associated with entropy production acts analogously to a source term in a continuity equation.

2.2 Quantum Thermodynamics

Having discussed some aspects of the essence of classical thermodynamics, we will now delve into quantum thermodynamics. To do this, we will begin our discussion by revisiting some elements of quantum mechanics, which can be found in various well-established literature such as [40, 41]. Next, we will define the usual notions of heat and work in quantum thermodynamics as in Ref.[15, 42].

In this context, let us consider a d-dimensional Hilbert space denoted by $\mathcal{H}^d$. In the context of Quantum Mechanics, the most general representation of a quantum system is made in terms of an operator, which we denote by $\rho \in L^1(\mathcal{H}^d)$ where $L^1(\mathcal{H}^d)$ denotes the space of Lebesgue measurable functions over the Hilbert space $\mathcal{H}^d$. Such an operator is associated with an ensemble $\{p_i, |\psi_i\rangle\}$, where p_i denotes the probability associated with each state $|\psi_i\rangle$ and carries all the information of a given physical system. Additionally, the following properties are satisfied by the density matrix operator ρ [41]:

(i) The density matrix ρ has trace equal to one.

(ii) The operator ρ is hermitian, i.e. $\rho = \rho^\dagger$.

(iii) The density matrix ρ is a positive operator.

The property (i) ensures the normalization of the density operator, (ii) guarantees that the eigenvalues of the density operator are real, while (iii) ensures the positivity of its elements. Furthermore, the elements of the density matrix ρ have certain relevant physical significance, especially in this work, to be discussed. In summary, the diagonal elements of ρ are real and are referred to as state populations or simply populations, which carry the physical information about the probabilities of the states, while the off-diagonal elements are called coherences [40, 41, 43].

In this sense, the most general form of density operator [41] is given by

$$\rho = \sum_j p_j \left|\psi_j\right\rangle \left\langle\psi_j\right| . \tag{2.14}$$

The density operator allows us to characterize a given state ρ as either pure or mixed. In particular, when $\mathrm{Tr}\left\{\rho^2\right\} = 1$, ρ is a pure state; on the other hand, if

$$\mathcal{P} = \mathrm{tr}\left(\rho^2\right) = \sum_j p_j^2 \leq 1,$$

ρ is called mixed state and $\mathcal{P}$ denote the purity of state. In particular, we can see that $\mathrm{Tr}\left\{\rho^2\right\}$ is bounded [41] as

$$\frac{1}{d} \leq \mathrm{tr}\left(\rho^2\right) \leq 1, \tag{2.15}$$

where $\frac{1}{d}$ occurs when we have the maximally disordered in the system which occurs where the density matrix is given by

$$\rho = \frac{\mathbb{1}_d}{d}, \tag{2.16}$$

where $\mathbb{1}_d$ denotes a $d \times d$ identity matrix.

Another important aspect in this scenario, is how the density operator evolves in time. In this sense, for a quantum system under unitary evolution, we have that the unitary evolution operator $U(t, t_0)$ satisfies the following initial value problem:

$$\begin{cases} i\dfrac{\partial}{\partial t} U\left(t, t_0\right) = H(t) U\left(t, t_0\right) \\ U(t_0, t_0) = \mathbb{1} \end{cases} \tag{2.17}$$

where $\mathbb{1}$ denotes the identity operator and $H(t)$ is the time-dependent Hamiltonian operator defined on $\mathcal{H}^d$. The most general solution of Eq. (2.17) is given by:

$$U\left(t, t_0\right)=\mathbb{1}+\sum_{j=1}^{\infty}\left(\frac{-i}{\hbar}\right)^j \int_{t_0}^t d t_1 \int_{t_0}^{t_1} d t_2 \cdots \int_{t_0}^{t_{j-1}} d t_n H\left(t_1\right) H\left(t_2\right) \cdots H\left(t_j\right). \tag{2.18}$$

A particular case of the system in Eq. (2.17) and, consequently, of the solution in Eq. (2.18) occurs when the Hamiltonian operator is time-independent. In this case, the problem in Eq. (2.17) reduces to a simple differential equation whose solution is given by:

$$U(t, t_0)=e^{-iH(t-t_0)}. \tag{2.19}$$

In particular, the set of evolution operators $U(t, t_0)$ forms a semigroup with respect to the usual multiplication operation between operators [40, 44].

With this, it follows that given a state at a time t_0 given by $\rho(t_0)$ the state at a time $t \geq t_0$ is given by:

$$\rho(t)=U\left(t, t_0\right) \rho\left(t_0\right) U^{\dagger}\left(t, t_0\right), \tag{2.20}$$

where $U(t, t_0)$ satisfies the problem in Eq. (2.17). The equality in Eq. (2.20) determines the time evolution of the density operator under unitary dynamics, however, we can still obtain a dynamic equation for the density operator. To this end, let us consider a system governed by a Hamiltonian $H(t)$ and consider the quantum states $\left|\psi_j(t_0)\right\rangle$ such that $\left|\psi_j(t)\right\rangle = U(t, t_0)\left|\psi_j(t_0)\right\rangle$. Then, from the density operator in the most general form given by Eq. (2.14) it follows that:

$$\begin{aligned}
i \frac{\partial \rho(t)}{\partial t} &= \sum_j\left(i \frac{\partial}{\partial t}\left|\psi_j(t)\right\rangle\right)\left\langle\psi_j(t)\right|+\left|\psi_j(t)\right\rangle\left(i \frac{\partial}{\partial t}\left\langle\psi_j(t)\right|\right) \\
&= \sum_j H(t)\left|\psi_j(t)\right\rangle\left\langle\psi_j(t)\right|-\left|\psi_j(t)\right\rangle\left\langle\psi_j(t)\right| H(t) \\
&= H(t) \rho(t)-\rho(t) H(t).
\end{aligned}$$

Therefore, we obtain the following equation:

$$\frac{\partial \rho(t)}{\partial t}=-i[H(t), \rho(t)] \tag{2.21}$$

which is called the Liouville-von Neumann equation [40] due to the similarity with respect to the Liouville equation that emerges in the context of classical mechanics [45].

The quantum dynamics given by Eq. (2.21) is established under the hypothesis that the evolution of the system is unitary, that is, the states evolve according to the Schrödinger equation.

However, even in non-relativistic quantum mechanics, this is not the most general scenario for describing the dynamics of the density operator, since in this regime we can have cases where the dynamics of the operator is non-unitary.

2.2.1 Work, heat and first law

From this, we can begin to introduce some important notions for quantum thermodynamics. In summary, the unitarity or non-unitarity of the system's dynamics, and consequently of the density operator, is a crucial aspect for defining closed and open systems in the context of quantum thermodynamics. Certainly, we say that a quantum system is closed as long as its dynamics are unitary, that is, described according to the Schrödinger Equation Eq. (2.17) or, equivalently, the Liouville-von Neumann Equation Eq. (2.21).

Furthermore, note that even a system with a time-dependent Hamiltonian, meaning the energy of the system is not conserved, is still said to be a closed system. This is particularly the case because we consider that the injection or removal of energy in the system is done in a sufficiently controlled manner so that the system can still be considered closed, which resembles the classical description of a piston that can move in the context of quantum thermodynamics.

Consequently, we say that a system is open if its evolution is non-unitary. In particular, this scenario occurs when we consider a quantum system, described by a Hamiltonian H_S, that interacts with an environment described by a Hamiltonian H_R. Therefore, the total Hamiltonian of the system is given by:

$$H = H_S \otimes \mathbb{I}_{\mathbb{R}} + \mathbb{I}_{\mathbb{S}} \otimes H_R + \epsilon H_I \tag{2.22}$$

where $\mathbb{I}_{\mathbb{R}}$ and $\mathbb{I}_S$ represents, in order, the identity operator in the Hilbert space associated to the environment $\mathcal{H}_R$ and the open system $\mathcal{H}_S$. The Hamiltonian H_I characterizes the interaction between S and R, the parameter ϵ characterizes the strength of the coupling of the interaction Hamiltonian.

The description provided by Eq. (2.22) is valid under weak coupling conditions, meaning the reservoir R is sufficiently large with an infinite number of degrees of freedom, the parameter ϵ is small, and the system-reservoir interaction is irreversible. In particular, under these assumptions we can derive the system's state dynamics, which becomes non-unitary as we trace out the reservoir's degrees of freedom. That is, the dynamics previously described by the Liouville-von Neumann equation Eq. (2.21) no longer holds under these conditions.

However, even under a non-unitary regime, it is still possible to describe the dynamics of the density operator. In summary, the evolution of this operator is then defined by the Lindblad

Master Equation [46] given by:

$$\begin{aligned} \frac{\mathrm{d}\,\rho(t)}{\mathrm{dt}} &= -i[H(t), \rho(t)] + \mathcal{D}[\rho(t)], & (2.23) \\ \mathcal{D}[\rho(t)] &= \sum_{k=1}^{d^2} \gamma_k \left(L_k \rho L_k^\dagger - \frac{1}{2} \left\{ L_k^\dagger L_k, \rho(t) \right\} \right) & (2.24) \end{aligned}$$

where $\mathcal{D}[\rho(t)]$ is called dissipator, and the right side of the equation Eq. (2.23) defines a linear superoperator $\mathcal{L}(\rho) \equiv -i[H(t), \rho(t)] + \mathcal{D}[\rho(t)]$ it is also customary to call $\mathcal{L}\{\rho\}$ the Liouvillian because the analogy betweeen Eq. (2.23) and the Liouville equation Eq. (2.21).

With these discussions, we now have the main results associated with the density operator in quantum mechanics, as well as the determination of concepts that define what we call closed and open systems in the context of quantum mechanics. So, let's now begin to define the notions of the main thermodynamic quantities in the context of the first law. In particular, the first definitions of heat and work in the context of quantum thermodynamics were made by Alicki [15].

Indeed, following the notions presented in [15], we define the internal energy of a system by the expected value of the Hamiltonian operator, i.e.:

$$\mathrm{U} = \langle H \rangle = \mathrm{Tr}\left\{ \rho(t) H(t) \right\}, \tag{2.25}$$

notice that we denote the energy of the system by U which differs from the notation used for the time evolution operator $U(t, t_0)$. From this, using the linearity of the trace functional, and taking the differential of the expression in Eq. (2.25) it follows that we have

$$\mathrm{d}\,\mathrm{U} = \mathrm{d}\,\mathrm{Tr}\left\{ \rho(t) H(t) \right\} = \mathrm{Tr}\left\{ \mathrm{d}\,\rho(t) H(t) \right\} + \mathrm{Tr}\{ \rho(t)\, \mathrm{d}\, H(t) \}. \tag{2.26}$$

The first term that appears in the last equality is what we associate with the differential contribution of heat to the system, while the second is what we associate with the differential of work.

Notice that the quantity we associate with work is connected to modifications in the Hamiltonian, which is well-behaved since we have a high level of controllability over quantum systems. On the other hand, the change in states is not something controllable; in summary, these changes emerge as responses to the modifications experienced by the system. Thus, these energy contributions are identified as heat, in analogy to the classical notion we discussed earlier.

Therefore, the notions of heat and work in quantum thermodynamics are expressed, in differential form, as:

$$\mathrm{d}\,Q_u[\rho(t)] = \mathrm{Tr}\{ H\, \mathrm{d}\,\rho \}, \tag{2.27}$$

$$\mathrm{d}\,W_u[\rho(t)] = \mathrm{Tr}\{ \mathrm{d}\,H \rho \}, \tag{2.28}$$

in which $Q_u[\rho(t)]$ and $W_u[\rho(t)]$ denote heat and work respectively, the subscript label u designates the word usual, which will be relevant in later chapters where we will introduce other notions of heat and work. More commonly, these quantities can be written as:

$$\begin{aligned} Q_u[\rho(t)] &= \int_0^\tau dt \, \mathrm{Tr}\left\{\frac{\mathrm{d}\,\rho(t)}{\mathrm{dt}} H(t)\right\}, \quad (2.29)\\ W_u[\rho(t)] &= \int_0^\tau dt \, \mathrm{Tr}\left\{\rho(t)\frac{\mathrm{d}\,H(t)}{\mathrm{dt}}\right\}, \quad (2.30)\end{aligned}$$

considering a dynamics defined such that $t \in [0, \tau]$ where τ is the time of evolution. Note that the notion of usual heat introduced in Eq. (2.30) reasonably agrees with the classical notion of work understood as the integral of a power function [42, 45]. With this, we can then formulate the first law of thermodynamics in the context of quantum thermodynamics, which is expressed, in differential form, by:

$$\mathrm{d}\,\mathrm{U} = \mathrm{d}\,W_u[\rho(t)] + \mathrm{d}\,Q_u[\rho(t)] \quad (2.31)$$

more usually:

$$\Delta\,\mathrm{U} = W_u[\rho(t)] + Q_u[\rho(t)] \quad (2.32)$$

since $W_u[\rho(0)] = Q_u[\rho(0)] = 0$ and $\Delta\,\mathrm{U} = \mathrm{U}(t) - \mathrm{U}(0)$.

The expressions for heat Eq. (2.29) and work Eq. (2.30) were obtained without any considerations regarding the nature of the dynamics of the density operator. Thus, these definitions remain valid both in the context of open systems and closed systems. In this sense, it is interesting to evaluate the behavior of heat in the particular case where we have a closed system. In this regime, the density operator evolves according to the Liouville-Von Neumann equation Eq. (2.21), thus, it follows that the heat Eq. (2.29) is such that

$$\begin{aligned} Q_u[\rho(t)] &= \int_0^\tau \mathrm{dt}\,\mathrm{Tr}\left\{\frac{\mathrm{d}\,\rho(t)}{\mathrm{dt}} H(t)\right\}\\ &= \int_0^\tau \mathrm{dt}\,\mathrm{Tr}\left\{-i[H(t),\rho(t)]H(t)\right\}\\ &= -i\int_0^\tau \mathrm{dt}\,\mathrm{Tr}\left\{[H(t),\rho(t)H(t)]\right\}\\ &= 0\end{aligned}$$

since the trace of any commutator is always zero, that is, $\mathrm{Tr}\{[A, B]\} = 0$ for all operators A and B. Consequently, this establishes a result analogous to what we have in classical thermodynamics: The heat involved in a given thermodynamic process, in a closed system, is always zero.

However, note that the heat introduced by Alicki is closely tied to the unitarity of the dynamics, particularly describing the energy exchange associated with the interaction between the system and a possible coupled bath. In this sense, the previous result indicates that this energy contribution is null in closed systems. Nevertheless, there are several other developments in quantum thermodynamics where notions of energy, analogous to heat, are introduced in closed systems. These contributions, in turn, can have different natures, such as being connected to "internal frictions" [23], non-adiabaticity in unitary dynamics [22], and even out-of-equilibrium processes [47]. In particular, these distinct contributions emerge in the quantum scenario through the production of uncertainties in energy measurements arising from the generation of quantum coherences in the energy basis [24].

In Chapter 4, we will discuss in more detail specific situations where energy contributions, more specifically parts of the work done on a system, can be interpreted as heat [3].

2.3 Different notions of entropy

In the previous section, we introduced the physical quantities associated with heat and work, as well as the first law of thermodynamics in the context of quantum mechanics. A natural continuation would then be to establish a notion of entropy and, consequently, establish a second law for quantum thermodynamics. However, the concept of entropy is one of the most debated and mystified in the history of science [25]. As a result, various schools of thought have emerged, leading to the concept of entropy being formulated with different notions both philosophical-conceptual and quantitative-numerical [48]. With this in mind, let us then discuss some notions of entropy that appear as candidates for microscopic entropy [25, 48].

2.3.1 Von Neumann entropy

The first definition of entropy that we will revisit is the so-called Von Neumann entropy, which usually appears as thermodynamic entropy [25, 49] and is defined by:

$$S_u[\rho] = -\,\mathrm{Tr}\left\{\rho\log(\rho)\right\}. \tag{2.33}$$

This entropy is associated to the minimization of Shannon entropy [50, 51] over all basis [52].

In this work, we reefears to the Von Neumann entropy as usual entropy. In fact, this entropy is consistent with thermodynamic entropy only in two cases

I) When the system is in equilibrium and is represented by statistical ensembles. For example, the Gibss thermal state given us:

$$\rho_G = \frac{e^{-\beta H}}{Z} \implies S_u[\rho_G] = -\sum_n E_n \log(E_n) \tag{2.34}$$

where β is the inverse of temperature and $Z \equiv= \mathrm{Tr}\{e^{-\beta H}\}$ is the partition function.

II) The second case is for ensembles even out of equilibrium that describes open systems coupled to an ideal heat bath.

The consideration that Von Neumann entropy is not, in general, a thermodynamic entropy is fundamentally important. Indeed, there are numerous works, especially in the realm of information theory, that employ its use as such without due concern for the precise conditions necessary for this attribution. With this in mind, we can cite, as an illustrative example, the case of an ideal gas undergoing free expansion, where the entropy increases during the expansion. However, free expansion is a reversible process, and thus the Von Neumann entropy in this process is zero, which does not correspond to the actual physical nature of the problem [53]. Furthermore, inconsistencies in the very derivation of entropies can also be observed when comparing the origin of the line elements associated with typically informational entropies and thermodynamic entropy.

The Von Neumann entropy possesses several particular properties, which we will now present. Indeed, these are:

(i) Von Neumann entropy is invariant under unitary transformation. In fact, consider a unitary transformation V then we have:

$$S_u[V\rho V] = -\,\mathrm{Tr}\left\{V\rho V^\dagger \log(V\rho V^\dagger)\right\} = \mathrm{Tr}\left\{V\rho \log(\rho) V^\dagger\right\} = S_u[\rho] \tag{2.35}$$

since, for every differential function F and a unitary transformation V we have $F(VxV^\dagger) = VF(x)V^\dagger$, and the last equality holds by cyclic property of the trace.

(ii) Von Neumann entropy is invariant in closed system. This follows immediately from the invariance under unitary transformation since that in closed system the evolution is unitary, then $\rho(t) = U(t,t_0)\rho(t_0)U^\dagger(t,t_0)$ which gives the time invariance:

$$S_u[\rho(t)] = S_u[U(t,t_0)\rho(t_0)U^\dagger(t,t_0)] = S_u[\rho(t_0)]. \tag{2.36}$$

(iii) Spectral decomposition of density operator in Von Neumann entropy. Since the density matrix ρ is a Hermitian operator, it can be spectrally decomposed as $\rho = \sum_k p_k \left|\psi_k\right\rangle \left\langle\psi_k\right|$, where $\{p_k\}$ is a set of eigenvalues and $\{\left|\psi_k\right\rangle\}$ is a set of corresponding eigenvectors that form an orthonormal basis. Using this decomposition in Von Neumann entropy we have

$$\begin{aligned}
S_u[\rho(t)] &= -\operatorname{Tr}\{\rho(t)\log[\rho(t)]\} \\
&= -\sum_j \langle\psi_j| \left[\sum_k p_k |\psi_k\rangle\langle\psi_k| \log\left(\sum_n p_n |\psi_n\rangle\langle\psi_n|\right)\right] |\psi_j\rangle \\
&= -\sum_{j,k} \langle\psi_j|\psi_k\rangle\, p_k \log\left(\sum_n p_n \langle\psi_k|\psi_n\rangle\langle\psi_n|\psi_j\rangle\right) \\
&= -\sum_k p_k \log(p_k)
\end{aligned}$$

then, we can write the Von Neumann entropy as

$$S_u[\rho(t)] = -\sum_k p_k \log(p_k) \tag{2.37}$$

where $p_k \in [0,1]$ since that ρ is a positive operator and his trace is equal to 1.

(iv) Von Neumann entropy is equal to zero if and only if $\rho(t)$ is a pure state, i.e.

$$S_u[\rho(t)] = 0 \iff \operatorname{Tr}\{\rho^2(t)\} = 1. \tag{2.38}$$

In fact, let us consider a normalized a quantum state $|\psi_k(t)\rangle$, and a orthonormal set $\{|\psi\rangle_j\}$ where $j = 1, ..., k, ...$ The density matrix associated to this pure state labeled by k is $\rho(t) = |\psi_k(t)\rangle\langle\psi_k(t)|$ therefore:

$$\begin{aligned}
S_u[\rho(t)] &= S_u[|\psi_k(t)\rangle\langle\psi_k(t)|] \\
&= -\operatorname{Tr}\{|\psi_k(t)\rangle\langle\psi_k(t)| \log[|\psi_k(t)\rangle\langle\psi_k(t)|]\} \\
&= -\sum_j \langle\psi_j| [|\psi_k(t)\rangle\langle\psi_k(t)| \log[|\psi_k(t)\rangle\langle\psi_k(t)|]] |\psi_j\rangle \\
&= -\langle\psi_k(t)| \log[|\psi_k(t)\rangle\langle\psi_k(t)|] |\psi_k\rangle \\
&= -\log[\langle\psi_k(t)\rangle\langle\psi_k(t)\rangle] \\
&= -\log(1) = 0
\end{aligned}$$

since the $|\psi_k(t)\rangle$ is normalized. For other hands, suppose, by contradiction, that $\rho(t)$ is a mixed state as Eq. (2.14) and $S_u[\rho(t)] = 0$ therefore, from (iii) we have

$$S_u[\rho(t)] = 0 \implies -\sum_k p_k \log(\rho_k) = 0 \implies p_k = 1$$

since $p_k \in [0,1]$. Therefore, if $S_u[\rho(t)] = 0$ the density operator is a pure state.

The Von Neumann entropy has a considerable number of other properties [41, 50]. The properties we highlighted and proved above are relevant in our discussion about a microscopic definition of thermodynamic entropy. Indeed, in the preceding discussions, we will always compare each entropy with the Von Neumann entropy, particularly concerning these properties.

2.3.2 Boltzman entropy

Another important definition of entropy is the Boltzmann entropy. Let us consider H be the Hamiltonnian of an isolated system where we drive any dependence on external paramater g_t. In this sense, the system is governerd by the following stationary Schrödinger equation:

$$H\left|E_i, l_i\right\rangle = E_i\left|E_i, l_i\right\rangle ,$$

where $\{\left|E_i, l_i\right\rangle\}$ correspond to the set of energy eigenstates with energy eigenvalues E_i and labels possible exact degeneraries.

Now, let us consider a scenario where our objective is to perform an energy measurement. Indeed, in the situation where our system is sufficiently simple and controllable such that the observer has full control of the experiment, any energy measurement can be understood in relation to the projection of each eigenenergy $\Pi_i = \left|E_i, l_i\right\rangle\left\langle E_i, l_i\right|$.

However, this is an ideal scenario, and certainly in more realistic systems, one may not have full control over the experiment such that there is some uncertainty δ associated with the ignorance of the energy measurement. In this sense, we have a scenario in which the energy measurement is then characterized by the following projector

$$\Pi_E = \sum_{E_i \in [E, E+\delta)} \sum_{\ell_i} \left|E_i, l_i\right\rangle\left\langle E_i, l_i\right| . \tag{2.39}$$

In fact, the uncertainty associated with the parameter δ is related to the observer's ignorance regarding some element of the system and/or the inherent impossibility of fine measurement in the conducted experiment. The projectors obtained by Eq. (2.39) form an orthogonal set such that the equalities:

$$\begin{cases} \Pi_E \Pi_{E'} = \delta_{E,E'} \Pi_E \\ \sum_E \Pi_E = \mathbb{1} \end{cases} \tag{2.40}$$

where $\delta_{E,E'}$ the Kronecker delta. In particular, sets of projectors that satisfy the equalities given in Eq. (2.40) define what we call a coarse-grained measurement. The most general case is when we have information about further macroscopic variables, such as the particle number N.

If a coarse-grained measurement results in outcome E, the Boltzmann entropy of the system is

$$S_B(E) \equiv \log(V_E), V_E \equiv \mathrm{Tr}\{\Pi_E\} = \dim\{\Pi_E\} \tag{2.41}$$

where V_E is referred as the system's volume element which is the rank of the projector Π_E.

When information about additional macroscopic variables, such as particle number N, is available, the Boltzmann entropy can be generalized as

$$S_B(E, N, ...) \equiv \log(V_{E,N,...}) \tag{2.42}$$

where $V_{E,N,...}$ counting all the microstate compatible with the macroscopic constraints $E, N, ...$

A particularly interesting case is to compare the Boltzmann entropy with the Von Neumann entropy, especially concerning the result of property Eq. (2.38). Indeed, let us consider a closed system that is governed by the following Hamiltonian:

$$H = \begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix}, \quad a \neq b \tag{2.43}$$

now, let's consider a pure state $\rho = |\psi\rangle\langle\psi|$ confined to an energy shell $[a, a+\delta)$ with δ being the imprecision in the energy measurement such that $\delta > b$. Consequently, we have that $[a, a+b] \subset [a, a+\delta)$, and therefore the projector Π_E is given by:

$$\pi_E = |a, 1\rangle\langle a, 1| + |b, 1\rangle\langle b, 1| \tag{2.44}$$

then, the Boltzmann entropy is given by:

$$S_B(E) = \log(V_E) = \log(\mathrm{Tr}\{\pi_E\}) = \log(2) \neq 0, \tag{2.45}$$

therefore, this simple case reveals the Boltzmann entropy is nonzero even for a pure state. In the case of the measuremeant is perfect i.e. $\delta = 0$ the Boltzmann entropy is zero if and only if the systems is non-degenerated.

Another interesting aspect of the Boltzmann entropy is related on how intuitively this entropy explain the second Law of thermodynamics without needing the notion of the statistical ensembles [26]. For an isolated system, the evolution towards a state of higher volume is statistically favored, resulting in the system spending a significant fraction of its time in the state of maximum volume. This state of maximum volume corresponds to thermodynamic equilibrium. This phenomenon explains the increase in entropy observed upon the removal of a constraint and the general tendency for systems to evolve towards a state of maximum entropy [26].

However, the dependence of the coarse-grained measurement in the Boltzmann entropy reveals some inadequacy in the description of small quantum systems, where an experimenter usually has precise control over the quantum degrees of freedom. In this case, the volume term V_E reduces to 1, and the description of Boltzmann entropy vanishes.

2.3.3 Observational entropy

The Von Neumann and Boltzmann entropy can be interpolated into another concept of entropy, which is called *observational entropy* [54]. This concept of entropy is defined in a general way based on the notion of a coarse-grained measurement, which we introduced in Eq. (2.40). In this sense, let us consider a general coarse-graining measurement defined by the set $\mathcal{C} = \{\Pi_c\}$ of orthogonal projectors that satisfy the same relations in Eq. (2.40). Therefore, for any system described by the state ρ (pure or mixed), the observational entropy is defined as:

$$S_{obs}^{\mathcal{C}}(\rho) \equiv -\sum_c p_c \log\left(\frac{p_c}{V_c}\right) \tag{2.46}$$

where $p_c \equiv \mathrm{Tr}\{\Pi_c \rho\}$ is the probability of observing the outcome c while $V_c \equiv \mathrm{Tr}\{\Pi_c\}$ is the volume term of Π_c. Specially, we can rewrite this entropy as:

$$S_{obs}^{\mathcal{C}} = -\sum_c p_c \log(p_c) + p_c \log(V_c) = S_{sh}\left(p_c\right) + \langle S_B(c)\rangle_{p_c}$$

where $S_{sh}\left(p_c\right) = -\sum_c p_c \log(p_c)$ is the Shannon entropy associated with the probabilities p_c and $\langle S_B(c)\rangle_{p_c}$ is the mean of the Boltzmann entropy.

The generality of the type of coarse-graining introduced in the definition of observational entropy allows us to restore the notions of Von Neumann and Boltzmann entropy as particular cases associated with when we have specific coarse-grainings. In effect, these cases correspond to the following:

I) When we have access to all physical information about the system, we can choose coarse-graining $\mathcal{C}_\psi = \{|\psi\rangle\langle\psi|\}$ correspondent to the eigenstate of the system's density operator $\rho = \sum_\psi \rho_\psi |\psi\rangle\langle\psi|$. In this case each volume term is equal to one, i.e. $V_\psi = 1$, therefore the observational entropy recalls:

$$S_{obs}^{\mathcal{C}_\psi}(\rho) = -\sum_\psi p_\psi \log\left(\frac{p_\psi}{V_\psi}\right) = S_{sh}(\rho) + \sum_\psi \langle p_\psi \log(V_\psi)\rangle = S_u(\rho), \tag{2.47}$$

this situation corresponds when the measuremant is the most informative possible.

II) The second case, which restore the Boltzmann entropy is associated where we only access to imprecise measuremnts, i.e. the set of coarse-graining is resctricted to the coarse-graning as $C_O = \{|o\rangle\langle o|\}$. Furthermore, after the measurement the system we will have full confidence that the system's state ρ is found in a given macrostate Π_m, therefore the probability p_o fall to be

$$p_o = \mathrm{Tr}\{|o\rangle\langle o|\,\rho\} = \langle O|\,\rho\,|O\rangle = \delta_{mo}$$

then, the observational entropy reduces to:

$$\begin{aligned} S_{obs}^{\mathcal{C}_O}(\rho) &= -\sum_o p_o \log\left(\frac{p_o}{V_o}\right) \\ &= S_{sh}(\rho) + \sum_o p_o \log(V_o) \\ &= \log(V_m) = S_B(\Pi_m) \end{aligned} \tag{2.48}$$

since $p_0 = \delta_{mo}$, it follows that $S_{\text{sh}}(\rho) = -\delta_{mo}\log(\delta_{mo}) = 0$. Here, $S_B(\Pi_m)$ denotes the Boltzmann entropy associated with the volume generated by the macrostate Π_m. On the other hand, when the choice of macroscopic observable O is the energy of the system, Eq. (2.48) corresponds to the Boltzmann entropy given in Eq. (2.41). Equivalently, if O corresponds to a set of observables, then Eq. (2.48) reduces to the general expression for Boltzmann entropy given in Eq. (2.42).

In summary, observational entropy provides us with a family of entropies, each associated with a type of coarse-graining measurement. However, notice that we have no indication of which coarse-graining measurement to choose or even any guiding criterion for such a choice. Certainly, such arbitrariness in its definition, which can be considered a major positive point for observational entropy, also becomes a negative point in its definition, since its connection with thermodynamic entropy necessarily requires an appropriate choice of coarse-graining measurement [25].

Nevertheless, even with such arbitrariness, it is still possible to obtain certain properties for observational entropy. In effect, consider a coarse-graining measurement $X = \{\Pi_x\}$; therefore, some of the properties of observational entropy are:

i) If the system is governed by the finite $d-$dimensional Hamiltonian defined in the Hilbert space $\mathcal{H}^d$ the observational entropy is bounded as

$$S_u(\rho) \leq S_{Obs}^{X}(\rho) \leq \log(d). \tag{2.49}$$

ii) The observational entropy is extensive in the limit where one expects it to be extensive. Consider a composite system in the decorrelated state $\rho = \rho_1 \otimes \cdots \otimes \rho_n$ and a composite coarse-graining $X = X_1 \otimes \cdots \otimes X_n$ with projectors $\Pi_{x_1} \otimes \cdots \otimes \Pi_{x_n}$. Then,

$$S_{\text{obs}}^{X}(\rho) = \sum_{j=1}^{n} S_{\text{obs}}^{X_j}(\rho_j) \tag{2.50}$$

iii) We have

$$S_{\text{obs}}^{X}(\rho) = S_u\left[\sum_x p_x \rho(x)\right] + \sum_x p_x D[\rho(x) \| \omega(x)]. \tag{2.51}$$

where $D[\cdot\|\cdot]$ denotes the Kullback-Leibler divergence,[1] which is defined by $D[\rho\|\sigma] = \text{Tr}\{\rho\log\rho - \rho\log\sigma\}$.

iv) We have $S_u(\rho) = S_{\text{obs}}^{X}(\rho)$ if and only if

$$\rho = \sum_x p_x \omega(x) \tag{2.52}$$

for an arbitrary set of probabilities p_x.

v) If $S_{\text{obs}}^{X_0}(0) = S_u[\rho(0)]$, then

$$\Delta S_{\text{obs}}^{X_t}(t) = S_{\text{obs}}^{X_t}(t) - S_{\text{obs}}^{X_0}(0) \geq 0. \tag{2.53}$$

These properties are all presented and proven in [25]. In fact, the property in item v) is substantially important in the context of observational entropy. Indeed, the second law of thermodynamics, both in closed and open systems, is formulated from the inequality in Eq. (2.53) considering the coarse-graining measurement given by projectors of the form Eq. (2.39).

2.3.4 Diagonal entropy

Finally, let's now revisit an important definition of entropy. To do this, consider the case where we have a closed system which is described by some time-dependent Hamiltonian $H(t)$. Then, we define the diagonal entropy or d-entropy of any state $\rho(t)$ by:

$$S_d[\rho(t)] \equiv -\sum_n \rho_{nn}^{E}(t) \log[\rho_{nn}^{E}(t)] \tag{2.54}$$

where the superscript E is associated of the instantaneous energy eigenbasis of the Hamiltonian $H(t)$.

---

[1] In Appendix A.2, we present fundamental elements and key results from quantum information theory, with a particular focus on the Kullback-Leibler divergence.

The diagonal entropy was first introduced in Ref. [28]. In special, this entropy can be rewrite as:

$$S_d[\rho(t)] = S_u[\rho^E_{diag}(t)] \tag{2.55}$$

where $\rho^E_{diag}(t)$ is the diagonal part of the state ρ in instantaneous energy eigenbasis. Notice that $\rho^E_{diag}(t)$ is obtained by erasing the elements outside the main diagonal. Consequently, the state obtained in this way necessarily depends on the energy basis, and therefore the property of the associated Von Neumann entropy of being invariant under unitary transformations does not apply in this case, i.e., $S_u[\rho^E_{diag}(t)] \neq S_u[\rho^E(t)]$.

One of the motivations pointed out by Polkovnikov in Ref.[28] for the definition of diagonal entropy is associated with some inherent problems related to Von Neumann entropy. To make this discussion somewhat clearer, let's discuss a problem presented in Ref.[22].

In effect, consider an observable $\mathcal{O}$ and a sufficiently complex system that was subject to a process which started and ended in a distant past, and eventually achieved some steady state as in

$$\rho^E(t) = \sum_{mn} \rho^E_{nm} e^{-i(E_m - E_n)t} \left|E_m\right\rangle \left\langle E_n\right| \tag{2.56}$$

where the Hamiltonian of the system H is such that $H\left|E_n\right\rangle = E_n\left|E_n\right\rangle$ for the final time-dependent Hamiltonian. By the ergodic hypothesis time average of any thermodynamic observable should be equivalent to the equilibrium ensemble average. Therefore, the average of the observable $\mathcal{O}(t)$ is given by

$$\overline{\langle \mathcal{O}(t) \rangle} \equiv \lim_{T\to\infty} \frac{1}{T} \int_0^T \mathrm{d}t \langle \mathcal{O}(t) \rangle, \tag{2.57}$$

where the total time dependence of the average of $\mathcal{O}$ is in the density operator. Then, we can expand the Eq.Eq. (2.57) as

$$\begin{aligned}
\overline{\langle \mathcal{O}(t) \rangle} &= \lim_{T\to\infty} \frac{1}{T} \int_0^T \mathrm{d}t \langle \mathcal{O} \rangle \\
&= \lim_{T\to\infty} \frac{1}{T} \int_0^T \mathrm{d}t \, \mathrm{Tr}\{\rho(t)\mathcal{O}\} \\
&= \lim_{T\to\infty} \frac{1}{T} \int_0^T \mathrm{d}t \sum_{mn} \rho^E_{nm} e^{-i(E_m - E_n)t} \left\langle E_n\right| \mathcal{O} \left|E_m\right\rangle \\
&= \sum_{mn} \rho_{nm} \mathcal{O}_{nm} \lim_{T\to\infty} \frac{1}{T} \int_0^T \mathrm{d}t \, e^{-i(E_m - E_n)t} \\
&= \sum_{mn} \rho^E_{nm} \mathcal{O}_{nm} \delta_{nm}
\end{aligned}$$

therefore, the time average of the observable $\mathcal{O}$ is:

$$\overline{\langle \mathcal{O}(t) \rangle} = \sum_n \rho^E_{nn} \mathcal{O}_{nn}, \tag{2.58}$$

which is dependent only on the time-independent diagonal elements of the density operator in the eigenbasis of the Hamiltonian. Thus, this development reveals that all relevant thermodynamic information in a measurement is completely present in the diagonal elements of ρ in the energy basis.

Consequently, since only the diagonal elements of the density operator become truly relevant for a thermodynamic measurement, it follows that we have two possibilities for the Von Neumann entropy, which are:

i) Von Neumann entropy contains additional information, which does not appear in any thermodynamic measurement,

ii) The time average of an observable is different from the time average of entropy for an equilibrium ensemble.

In both cases, we see that the Von Neumann entropy faces difficulties in providing a correct description that would be physically expected.

In all these developments, it is always assumed that the Hamiltonian spectrum is non-degenerate, or if it is degenerate, these degeneracies are not relevant to the system. Thus, we can then interpret this entropy as a physical quantity that quantifies the amount of randomness observed in the energy basis of the system [28]. Specifically, diagonal entropy can be identified as measuring the total amount of information lost to a limited set of evaluable measurements.

Also in Ref.[28], several properties of diagonal entropy are presented and demonstrated. In effect, many of these properties confer a thermodynamic character to this entropy, among which we list some below.

i) $S_d[\rho(t)] = S_u[\rho(t)]$ if the state $\rho(t)$ is stationary (diagonal).

ii) We can define the relative entropy of coherences by:

$$\mathcal{C} \equiv S_d[\rho(t)] - S_u[\rho(t)] \tag{2.59}$$

which quantifies the amount of entropy that is "lost" when the coherence elements are ignored.

iii) If the initial state is stationary then for any time-dependent process in a closed Hamiltonian system we have

$$S_d[\rho(t)] \geq S_d[\rho(0)] \tag{2.60}$$

iv) Diagonal entropy respect the fundamental thermodynamic relation

$$\Delta \mathrm{U} = T\Delta S - \sum_j \left.\frac{\partial \mathrm{U}}{\partial \lambda_j}\right|_S \Delta\lambda_j, \tag{2.61}$$

which is given by:

$$\Delta \mathrm{U} = \sum_j \left.\frac{\partial \mathrm{U}}{\partial \lambda_j}\right|_{S_d} \Delta\lambda_j, \tag{2.62}$$

which is direct consequence f the thermodynamic postulate that require the entropy to be a unique function of energy E and the external parameters λ_j.

Formally, all this property is also proved in Ref.[28]. Here, I will give special attention to property iv), which can be obtained by expanding the system's energy as:

$$\Delta \mathrm{U} = \sum_n \rho_{nn}(t)E_n(t) \approx \sum_n \Delta E_n(t)\rho_{nn}(0) + \sum_n E_n(0)\Delta\rho_{nn}(t) \tag{2.63}$$

where $\Delta E_n(t) = E_n(t) - E_n(0)$ is the change in the instantaneous energy eigenstates due to the time evolution while $\Delta\rho_{nn}(t) = \rho_{nn}(t) - \rho_{nn}(0)$ is the change in the diagonal component of ρ in energy eigenbasis. In Ref.[22] Polkovnikov identifies the terms contained in the Eq. (2.63) as:

- The first term in Eq. (2.63) is:

  $$\Delta E_{ad} \equiv \sum_n \Delta E_n(t)\rho_{nn}(0) \tag{2.64}$$

  which is the adiabatic change of the system's energy, i.e. the work done by the system due to the changes of the external parameters λ_i.

- The second term in Eq. (2.63) is

  $$Q(t) \equiv \sum_n E_n(0)\Delta\rho_{nn}(t) \tag{2.65}$$

  which correspond to the non-adiabatic change of the energy, i.e. the heat generated by the system when the process is non-quasi-static.

Another property and discussion of the diagonal entropy can be found in Ref.[28].

In this sense, the diagonal entropy can be connected to the notions of work and heat. Specifically, the heat introduced in Eq. (2.65) appears in both open and closed systems, which contradicts the usual definition of heat that we introduced in Eq. (2.29). In effect, the heat term introduced by Polkovnikov initially in Ref.[22] is associated with changes in the energy basis that are not adiabatic and can occur even in closed systems. Consequently, it is directly linked to the entropy of the system and is non-negative if the system starts in some equilibrium state [22, 24].

Chapter 3

Gauge invariant quantum thermodynamics: Foundations

This chapter introduces the fundamental concepts associated with the principle of gauge invariance in the context of quantum thermodynamics. In this sense, we begin by providing a concise overview of gauge theories, both within the framework of physics and as a mathematical theory. Specifically, we will initially present classical electrodynamics as a foundational example and motivation for the principle of gauge invariance.

Subsequently, the remaining sections of this chapter focus on review of the work of Céleri and Rudnicki [3] over gauge-invariant quantum thermodynamics, along with generalizations of some specific aspects of this work. This involves constructing the emergent gauge group and establishing the principle of gauge invariance inspired by the fundamental concepts of gauge theory, as discussed in the first section.

With the emergent gauge group defined, we introduce the concept of invariant quantities, in context of quantum thermodynamics, that form the invariant space associated with the emergent gauge group in quantum thermodynamics.

Here, two generalization are employed with respect to the development in [3], they are:

- We consider the system has arbitrary number of the degeneracies which can changes in relation a specific one parameter (time),
- The definition of invariant quantities is reformulated for a general case of the Haar average.

3.1 Brief overview of gauge theories

The principle of gauge or gauge invariance is a strong mathematical principle that underlies several physical theories, for example, the standard model of particle physics. In effect, gauge invariance emerges in physical theories, especially in field theories, from some mathematical redundancy associated with their descriptions, which allows for the introduction of sets of transformations that leave the equations of motion of the theory invariant. Among the theories that exhibit gauge invariance, we can mention classical electrodynamics.

Classical electrodynamics is a classical field theory that describes the interaction and evolution of electric fields $\vec{E}(\vec{x},t)$ and magnetic fields $\vec{B}(\vec{x},t)$ as well as their temporal evolutions. In effect, such a description is provided by a set of equations, namely the four Maxwell's equations, along with the continuity equation for the volume charge density $\rho(\vec{x},t)$ and volume current density $\vec{J}(\vec{x},t)$, which, in the absence of magnetic monopoles, are given by:

$$\text{Coulomb's law:} \qquad \vec{\nabla}\cdot\vec{D}(\vec{x},t) = \rho(\vec{x},t) \tag{3.1}$$

$$\text{Ampère's law:} \qquad \vec{\nabla}\times\vec{H}(\vec{x},t) - \frac{\partial\vec{D}(\vec{x},t)}{\partial t} = \vec{J}(\vec{x},t) \tag{3.2}$$

$$\text{Faraday's law:} \qquad \vec{\nabla}\times\vec{E}(\vec{x},t) + \frac{\partial\vec{B}(\vec{x},t)}{\partial t} = \vec{0} \tag{3.3}$$

$$\text{Absence of free magnetic poles:} \qquad \vec{\nabla}\cdot\vec{B}(\vec{x},t) = 0 \tag{3.4}$$

$$\text{Continuity equation:} \qquad \frac{\partial\rho(\vec{x},t)}{\partial t} + \vec{\nabla}\cdot\vec{J}(\vec{x},t) = 0 \tag{3.5}$$

in the S.I system. Here, $\vec{D}(\vec{x},t)$ and $\vec{H}(\vec{x},t)$ are the displacement electric field and magnetic field respectively. Furthermore, in classical electrodynamics we have two others essentials elements wich emerges from the Maxwell equations. In fact, from absence of free magnetic poles we have

$$\vec{\nabla}\cdot\vec{B}(\vec{x},t) = 0 \quad\Longrightarrow\quad \exists\,\vec{A}(x,t)\ e.g.,\ \vec{B}(\vec{x},t) = \vec{\nabla}\times\vec{A}(x,t) \tag{3.6}$$

where $\vec{A}(\vec{x},t)$ is called vector potential. From Faraday's Law,

$$\begin{aligned}
\vec{0} &= \vec{\nabla}\times\vec{E}(\vec{x},t) + \frac{\partial\vec{B}(\vec{x},t)}{\partial t} \\
&= \vec{\nabla}\times\vec{E}(\vec{x},t) + \frac{\partial\vec{\nabla}\times\vec{A}(x,t)}{\partial t} \\
&= \vec{\nabla}\times\left(\vec{E}(\vec{x},t) + \frac{\partial\vec{A}(x,t)}{\partial t}\right)
\end{aligned}$$

then, exists a scalar function $\Phi(x,t)$ such that:

$$-\vec{\nabla}\Phi(\vec{x},t) = \vec{E}(\vec{x},t) + \frac{\partial\vec{A}(x,t)}{\partial t} \;\Longrightarrow\; \vec{E}(\vec{x},t) = -\vec{\nabla}\Phi(\vec{x},t) - \frac{\partial\vec{A}(x,t)}{\partial t} \tag{3.7}$$

where $\Phi(\vec{x},t)$ is called scalar potential. Then, the equations (3.6) and (3.7) define the fields $\vec{E}(\vec{x},t)$ and $\vec{B}(\vec{x},t)$ in terms of a pair of potentials $\{\Phi(\vec{x},t),\vec{A}(\vec{x},t)\}$. However, the mathematical formulation of these two differential equations establishes a redundancy in the determination of the fields under a specific transformation of the potentials. This transformation is called a gauge transformation and is given by

$$\begin{cases} \Phi(\vec{x},t) \to \Phi'(\vec{x},t) = \Phi(\vec{x},t) - \dfrac{\partial \alpha(\vec{x},t)}{\partial t} \\ \vec{A}(\vec{x},t) \to \vec{A}'(\vec{x},t) = \vec{A}(\vec{x},t) + \vec{\nabla}\alpha(\vec{x},t) \end{cases} \tag{3.8}$$

where $\alpha(\vec{x},t)$ is a scalar function (real or not) of class $C^{\geq 2}$. In fact, using the transformed potentials we can see that the fields $\vec{E}'(\vec{x},t)$ and $\vec{B}'(\vec{x},t)$ (where the superscript ' denote the fields with the potentials $\Phi'(\vec{x},t)$ and $\vec{A}'(\vec{x},t)$) are equivalent to the fields $\vec{E}(\vec{x},t)$ and $\vec{B}(\vec{x},t)$. In another words, the fields are invariant under this transformation, indeed we proof it below, for the magnetic field:

$$\begin{aligned} \vec{B}'(\vec{x},t) &= \vec{\nabla} \times \vec{A}'(\vec{x},t) \\ &= \vec{\nabla} \times \left(\vec{A}(\vec{x},t) + \vec{\nabla}\alpha(\vec{x},t)\right) \\ &= \vec{\nabla} \times \vec{A}(\vec{x},t) + \vec{\nabla} \times \left(\vec{\nabla}\alpha(\vec{x},t)\right) \\ &= \vec{\nabla} \times \vec{A}(\vec{x},t) \\ &= \vec{B}(\vec{x},t), \end{aligned}$$

and for the electric field:

$$\begin{aligned} \vec{E}'(\vec{x},t) &= -\vec{\nabla}\Phi'(\vec{x},t) - \frac{\partial}{\partial t}\vec{A}'(\vec{x},t) \\ &= -\vec{\nabla}\left(\Phi(\vec{x},t) - \frac{\partial \alpha(\vec{x},t)}{\partial t}\right) - \frac{\partial}{\partial t}\left(\vec{A}(\vec{x},t) + \vec{\nabla}\alpha(\vec{x},t)\right) \\ &= -\vec{\nabla}\Phi(\vec{x},t) - \frac{\partial \vec{A}(\vec{x},t)}{\partial t} \\ &= \vec{E}(\vec{x},t). \end{aligned}$$

Therefore, the gauge transformations of the potentials doesn't modify the physics of the electrical and magnetic field. In reality, the function $\alpha(\vec{x},t)$ merely introduces redundancy in the determination of the potentials. Thus, we can then impose a specific constraint on each potential, or even on both, such that the function $\alpha(\vec{x},t)$ is determined to satisfy this constraint, which is commonly referred to as a gauge. Fixing the function $\alpha(\vec{x},t)$, or equivalently, fixing the gauge, eliminates all redundancies in the description. In addition, when we can ensure that the function $\alpha(\vec{x},t)$ satisfies this gauge, we say that the gauge is realizable.

In this sense, go to a practical example. Let us consider the Lorenz gauge:

$$\vec{\nabla} \cdot \vec{A}(\vec{x},t) + \frac{1}{c^2}\frac{\partial \Phi(\vec{x},t)}{\partial t} = 0. \tag{3.9}$$

In addition, consider a pair of potentials $\{\Phi_1(\vec{x},t), \vec{A}_1(\vec{x},t)\}$ that do not satisfy the Lorenz gauge

(3.9). Therefore, the Lorenz gauge can be realizable by a gauge transformation (3.8), then we have:

$$\begin{aligned} 0 &= \vec{\nabla}\cdot\vec{A}_1'(\vec{x},t) + \frac{1}{c^2}\frac{\partial\Phi_1'(\vec{x},t)}{\partial t} \\ &= \vec{\nabla}\cdot\left(\vec{A}_1(\vec{x},t) + \vec{\nabla}\alpha(\vec{x},t)\right) + \frac{1}{c^2}\frac{\partial}{\partial t}\left(\Phi_1(\vec{x},t) - \frac{1}{c^2}\frac{\partial\alpha(\vec{x},t)}{\partial t}\right) \\ &= \left(\vec{\nabla}\cdot\vec{A}_1(\vec{x},t) + \frac{1}{c^2}\frac{\partial\Phi_1(\vec{x},t)}{\partial t}\right) + \left(\nabla^2\alpha(\vec{x},t) - \frac{1}{c^2}\frac{\partial^2\alpha(\vec{x},t)}{\partial t^2}\right) \end{aligned}$$

thus, the function $\alpha(\vec{x},t)$ satisfy the following differential equation

$$\left(\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right)\alpha(\vec{x},t) = -\left(\vec{\nabla}\cdot\vec{A}_1(\vec{x},t) + \frac{1}{c^2}\frac{\partial\Phi_1(\vec{x},t)}{\partial t}\right). \tag{3.10}$$

This results in a non-homogeneous D'Alembert wave equation for $\alpha(\vec{x},t)$, where the non-homogeneous term arises from the contributions of the potentials. Since $\alpha(\vec{x},t)$ satisfy the equation (3.10), the Lorenz gauge is achievable for a gauge transformation of the potential pair $\{\Phi_1(\vec{x},t), \vec{A}_1(\vec{x},t)\}$.

Another interesting aspect to the gauge transformation defined in (3.8) is associated to the group theory. In the literature, the gauge redundancy of the fields, arising from the transformation of the potentials (3.8), is often referred to as gauge symmetry. In fact, the gauge symmetry it is not a symmetry of the system in the sense that it takes one physical state to a different physical state. Instead, it is a redundancy in our mathematical description of the system.

However, the gauge transformation (3.8) can be associated with the notion of symmetry established by group theory. In this context, the symmetry perspective is introduced by the group formed by all elements that satisfy the transformation (3.8), which, in the case of electrodynamics, corresponds to the group of unitary transformations $\mathcal{U}(1)$.

In this sense, we will demonstrate that the transformation of the potentials and their components under an arbitrary transformation of the $\mathcal{U}(1)$ group is given by (3.8). To this end, we will introduce the four-potential notation $A_\mu(\vec{x},t) = \left(\Phi(\vec{x},t), \vec{A}(\vec{x},t)\right)$ and the derivative operator $\partial_\mu = \left(-\frac{1}{c^2}\frac{\partial}{\partial t}, \vec{\nabla}\right)$, which are more commonly used for treating classical electrodynamics as a gauge theory. Within the context of the unitary group $\mathcal{U}(1)$, the most general element can be expressed as $\Omega(\vec{x},t) = e^{-\alpha(\vec{x},t)}$, where $\alpha(\vec{x},t)$ is an arbitrary complex scalar function. The transformation of each component of the four-vector potential under a $\mathcal{U}(1)$ transformation is then given by:

$$\begin{aligned} A_\mu(\vec{x},t) \to A_\mu'(\vec{x},t) &= \Omega(\vec{x},t)\left(A_\mu(\vec{x},t) + \partial_\mu\right)\Omega^{-1}(\vec{x},t) \\ &= e^{-\alpha(\vec{x},t)}\left(A_\mu(\vec{x},t) + \partial_\mu\right)e^{\alpha(\vec{x},t)} \\ &= e^{-\alpha(\vec{x},t)}A_\mu(\vec{x},t)e^{\alpha(\vec{x},t)} + e^{-\alpha(\vec{x},t)}\partial_\mu e^{\alpha(\vec{x},t)} \\ &= A_\mu(\vec{x},t) + \partial_\mu\alpha(\vec{x},t), \end{aligned} \tag{3.11}$$

which is equivalently with the gauge transformation defined in (3.8).

Therefore, since they gauge transformation of the potentials are can be written as a unitary transformation follows that the gauge transformations of the potentials that ensure the invariance of the fields $\vec{E}(\vec{x},t)$ and $\vec{B}(\vec{x},t)$ under Maxwell's equations are given by the $\mathcal{U}(1)$ group. This analysis establishes a elegant results: the electrodynamics as a abelian gauge theory which respect to the unitary group $\mathcal{U}(1)$.

This invariance is not limited in over the fields in electrodynamics. Indeed, other structures in electrodynamics are also invariant under transformations of the type described in Eq. (3.11). In this sense, we define the eletromagnetic tensor by the following relation:

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu. \tag{3.12}$$

For notational simplicity, i will henceforth omit the arguments $(\vec{x},t)$ from the potentials and fields. Then, we can write the field components as

$$E_i = F_{0i} \quad \text{and} \quad B_i = -\frac{1}{2}\epsilon_{ijk}F_{jk}, \tag{3.13}$$

where ϵ_{ijk} is the levi-civita symbol [55]. Furthermore, we also introduce the Lagrangian $\mathcal{L}$ and the action S, respectively, as:

$$\begin{aligned} \mathcal{L}\left(A_\mu, \partial_\nu A_\mu\right) &= -\frac{1}{4}F_{\mu\nu}F^{\mu\nu} - ej^\mu A_\mu, && (3.14) \\ S &= \int_{\mathbb{R}^{1,3}} \mathrm{d}^4\mathrm{x}\, \mathcal{L}\left(A_\mu, \partial_\nu A_\mu\right) && (3.15) \end{aligned}$$

where the measure $\mathrm{d}^4\mathrm{x}$ is associated with the temporal component $x^0 = t$ and the spatial components $\vec{x} = (x^1, x^2, x^3)$.

Using the gauge transformation for the four-vector A_μ given in Eq. (3.11), we can show that both the Maxwell tensor and the action remain invariant over this gauge transformation. Indeed, for the Maxwell tensor we have:

$$\begin{aligned} F_{\mu\nu}(A'_{\mu\nu}) &= \partial_\mu A'_\nu - \partial_\nu A'_\mu \\ &= \partial_\mu\left(A_\nu + \partial_\nu\alpha\right) - \partial_\nu\left(A_\mu + \partial_\mu\alpha\right) \\ &= \partial_\mu A_\nu - \partial_\nu A_\nu + \partial_\mu\partial_\nu\alpha - \partial_\nu\partial_\mu\alpha \\ &= \partial_\mu A_\nu - \partial_\nu A_\mu = F_{\mu\nu}\left(A_{\mu\nu}\right) \end{aligned}$$

and for the Action, we have

$$\begin{aligned}
S\left[A'\right] &= \int_{\mathbb{R}^{1,3}} \mathrm{d}^4\mathrm{x}\, \mathcal{L}\left(A'_\mu, \partial_\nu A'_\mu\right) \\
&= \int_{\mathbb{R}^{1,3}} \mathrm{d}^4\mathrm{x} \left[-\frac{1}{4} F_{\mu\nu}\left(A'\right) F^{\mu\nu}\left(A'\right) - e j^\mu \left(A'_\mu\right)\right] \\
&= \int_{\mathbb{R}^{1,3}} \mathrm{d}^4\mathrm{x} \left[-\frac{1}{4} F_{\mu\nu}\left(A'\right) F^{\mu\nu}\left(A'\right) - e j^\mu \left(A_\mu + \partial_\mu \alpha\right)\right] \\
&= \int_{\mathbb{R}^{1,3}} \mathrm{d}^4\mathrm{x} \left[-\frac{1}{4} F_{\mu\nu}(A) F^{\mu\nu}(A) - e j^\mu \left(A_\mu + \partial_\mu \alpha\right)\right] \qquad (3.16) \\
&= \int_{\mathbb{R}^{1,3}} \mathrm{d}^4\mathrm{x} \left[-\frac{1}{4} F_{\mu\nu} F^{\mu\nu} - e j^\mu A_\mu\right] - e \int_{\mathbb{R}^{1,3}} \mathrm{d}^4\mathrm{x} \left[j^\mu \partial_\mu \alpha\right] \qquad (3.17) \\
&= S[A] - e \int_{\mathbb{R}^{1,3}} \mathrm{d}^4\mathrm{x} \left[j^\mu \partial_\mu \alpha\right] = S[A], \qquad (3.18)
\end{aligned}$$

note that, in this development, the transformation of the four-vector $A_\mu(\vec{x}, t)$ under the action of the $\mathcal{U}(1)$ group generates, in the action S, a term associated with the components of the four-current j^μ, connected to the phase α that characterizes the group. However, using the invariance of the Maxwell tensor, previously demonstrated, we obtain Eq. (3.16), and consequently, Eq. (3.17) is naturally derived, allowing the identification of its first term as the action associated with the four-potential A. Furthermore, the invariance of the action under the $\mathcal{U}(1)$ group is then achieved by showing that the integral associated with the current j^μ and the phase α in Eq. (3.18) vanishes. Indeed, we detail this result below:

$$\begin{aligned}
\int_{\mathbb{R}^{1,3}} \mathrm{d}^4\mathrm{x} \left[j^\mu \partial_\mu \alpha\right] &= \int_{\mathbb{R}^{1,3}} \mathrm{d}^4\mathrm{x} \left[\partial_\mu (j^\mu \alpha) - \alpha \partial_\mu j^\mu\right] \\
&= \int_{\partial\mathbb{R}^{1,3}} d\Sigma [j^\mu \alpha] - \int_{\mathbb{R}^{1,3}} \mathrm{d}^4\mathrm{x} \left[\alpha (\partial_\mu j^\mu)\right] = 0, \qquad (3.19)
\end{aligned}$$

where we integrated by parts in the first line above and then applied the generalized Stokes theorem, so that the volume integral of $\partial_\mu (j^\mu \alpha)$ over $\mathbb{R}^{1,3}$ can be written as an integral over the boundary of $\mathbb{R}^{1,3}$, denoted by $\partial\mathbb{R}^{1,3}$, whose measure is denoted by $d\Sigma$. However, it is assumed that the components j^μ have finite support, i.e., they are defined over a subregion of $\partial\mathbb{R}^{1,3}$ with finite measure. As a result, the first integral in Eq. (3.19) vanishes. On the other hand, the second integral in Eq. (3.19) vanishes due to the continuity equation, i.e., $\partial_\mu j^\mu = 0$.

Notice that the result established by the invariance of the action under gauge transformations of the group $\mathcal{U}(1)$ is even stronger than just the invariance of the fields. Indeed, besides ensuring the invariance of the equations of motion, this result also provides us with the existence of a conserved quantity Q (charge) due to Noether's Theorem.

The invariance of electrodynamics under gauge transformations of the group $\mathcal{U}(1)$ was generalized by Yang and Mills in Ref. [56]. In this work, Yang and Mills provided an explanation for the conservation of isospin in collisions involving strong interactions based on the invariance of motion equations over the transformations of the group $\mathcal{SU}(2)$ [56]. The transformations of the group $\mathcal{SU}(2)$ do not commute with each other like the transformations of the group $\mathcal{U}(1)$ and therefore are called non-abelian. Furthermore, the family of gauge theories over the group $\mathcal{SU}(d)$ is called Yang-Mills theories.

The work of Yang-Mills for the strong interaction is a historical milestone for physics and especially for modern gauge theories [57]. In fact, this work did not have much relevance when first published in 1954, however, it pointed directions for a formulation of a gauge theory capable of explaining the mechanism of spontaneous symmetry breaking [58–60] which was initially proposed by Anderson in Ref.[61] in 1960. The explanation of the mechanism occurred in 1964 simultaneously by several independent groups [58, 59].

In this same decade, more precisely in 1961, Glashow in Ref.[62] proposed a theory for weak and electromagnetic interaction based on a gauge theory with symmetry $\mathcal{SU}(2)\times\mathcal{U}(1)$ where the groups $\mathcal{SU}(2)$ and $\mathcal{U}(1)$ are associated with weak and electromagnetic interactions, respectively. Glashow's initial proposal had some weaknesses, in particular, the Higgs mechanism was not included in his description. However, in 1967 and 1968, physicists Steven Weinberg [63] and Abdus Salam [64] incorporated the description of the Higgs mechanism into Glashow's theory and thus achieved the unification of weak and electromagnetic interactions in the so-called electroweak theory as a gauge theory associated with the non-abelian symmetry group $\mathcal{SU}(2) \times \mathcal{U}(1)$ [63, 64][1].

Moreover, the strong interaction has also been described as a gauge theory. In summary, the current description of the strong interaction that we know today as quantum chromodynamics (QCD) has gone through various works [65], particularly regarding which symmetry group the

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[1] A reader with some knowledge of field theory should note that here we are identifying the weak interaction in a simplified manner with respect to the associated gauge group. In fact, the group $\mathcal{U}(1)$ here is not exactly the same unitary group as in electrodynamics, which we will denote as $\mathcal{U}_{\text{em}}(1)$, but rather the unitary group associated with the weak hypercharge (Y), which we will denote by $\mathcal{U}_Y(1)$, while the special group will be denoted by $\mathcal{SU}_L(2)$, since the gauge transformations act only on left-handed fermions (and right-handed antifermions). Thus, in a simplified way, what the Higgs mechanism does is, under certain conditions, spontaneously break the gauge symmetry of the group $\mathcal{SU}_L(2)\times U(1)_Y \to \mathcal{U}_{\text{em}}(1)$ when the Higgs field (a doublet of $\mathcal{SU}_L(2)$ with weak hypercharge $Y = 1$, whose first component is charged while the second is neutral) acquires a non-zero Vacuum Expectation Value (VEV). This arises from the fact that the Higgs field is not invariant under all transformations of the group $\mathcal{SU}_L(2) \times U(1)_Y$, but it is invariant under all transformations of the group $\mathcal{U}_{\text{em}}(1)$. In this sense, after symmetry breaking, the original 4 massless vector bosons (which constitute the relevant degrees of freedom of the system when the Higgs field has a zero VEV) of the electroweak interaction combine to form new effective vector bosons, in particular, the photon, which is constituted by a linear combination of the original massless vector bosons, corresponding also to the symmetric phase of the primordial electroweak interaction. However, in addition to the massless photon, there are three other massive combinations that emerge in this mechanism, which acquire mass proportional to the VEV of the Higgs field: the W^+ and W^- bosons (responsible for mediating the charged weak interaction) and the Z^0 boson (responsible for mediating the neutral weak interaction). Thus, the photon and the massive vector bosons W^+, W^-, and Z^0 are the relevant vector bosonic degrees of freedom in the broken phase of the electroweak interaction, where the weak and electromagnetic interactions manifest in very different ways. The idea behind the proposed unification initially refers to an informal description that often originates from the fact that the electric charge observed today, associated with the gauge group $\mathcal{U}_{\text{em}}(1)$ of electromagnetism, can be written as a non-linear combination of the couplings g^L of the group $\mathcal{SU}_L(2)$ and g^Y of the group $\mathcal{U}_Y(1)$.

theory should be associated with; however, the group $\mathcal{SU}(3)$ has always been a strong candidate for the theory [66–69]. In fact, it was in Ref.[70] that physicists Gell-Mann, Fritzsch, and Heinrich Leutwyler conceived QCD as a gauge theory associated with the group $\mathcal{SU}(3)$.

The unification of the strong and electroweak interactions resulted in the formulation of the standard model of particle physics, which is a gauge theory associated with the non-abelian group $\mathcal{U}(1) \times \mathcal{SU}(2) \times \mathcal{SU}(3)$ [71].

Indeed, the fundamental field theories are strongly based on gauge invariance and consequently on the employment of symmetry groups for the description of the theory. Additionally, the formulation of a theory from a gauge invariance also provides a pathway for a geometric formulation of the theory. This perspective is associated with the fact that symmetry groups are Lie groups, i.e., differential manifolds equipped with group structures [72].

In particular, from a mathematical point of view, a gauge theory is the study of connections in vector or principal bundles (vector spaces associated with each point of the manifold) that satisfy some gauge invariant curvature condition in the manifold associated with the group [73, 74]. This group is called the gauge group, and in the most general scenario of gauge theories, the potentials A and the tensors F transform under the gauge transformation

$$A_\mu \;\rightarrow\; A'_\mu = V A_\mu V^{-1} + V \partial_\mu V^{-1} \tag{3.20}$$

$$F_{\mu\nu} \;\rightarrow\; F'_{\mu\nu} = V F_{\mu\nu} V^{-1} \tag{3.21}$$

where V is one element of the gauge group. If we choose $V = e^{i\alpha} \in \mathcal{U}(1)$, we obtain the same result expressed in Eq. (3.11), which is a particular case, restricted to the unitary group, of how gauge transformations act on the potentials. From a geometric perspective, the potentials A and the tensors F correspond to connections and curvatures, respectively, associated with the variety of the gauge group.

Thus, gauge theories are established on the solid mathematical framework of Lie group theory [72, 75] and, consequently, in differential geometry and topology [74, 76].

3.2 Thermodynamic gauge group

Now, we will develop the main notions for our formalism, with the notions of gauge transformation and gauge group being the first elements that we will seek to develop. In summary, this section follows the ideas initially proposed by Céleri and Rudnicki [3]. However, the formalism developed in this article is limited to a particular case where the spectrum of the Hamiltonian of the system is non-degenerate. Next, we will develop the entire formulation without this hypothesis.

First of all, it is important to emphasize that classical and/or quantum thermodynamics is not a gauge theory as we presented in the previous section. Indeed, their mathematical formulations do not involve the introduction of redundancies as discussed in Section 3.1. However, it is possible to formulate a notion of gauge invariance for the theory in an emergent manner from the intrinsic nature of the measurement processes that are performed in classical thermodynamics.

In fact, as we already discussed in Section 2.1, the precise description of all the constituents of a thermodynamic system, in the classical context, would involve solving a system of differential equations on the order of 10^{23} equations. But, this set of equations are the Newton's law is a second order ordinary differential equation which have the unique solution since the initial position and velocity of all therms are known, this its is a simple application of the Theorem of existence and uniqueness for ODEs [77].

However, obtaining solutions to these equations is computationally unfeasible, and the exact description of this macroscopic system, by the Newton's law, are impossible due to our computational limitation even though this solution exists and are unique.

Therefore, from this limitation the thermodynamics are developed over the fact of macroscopic measurements are extremely slow on the atomic scale of time, and they are extremely coarse grained on the atomic scale of distance [5]. In special, a macroscopic observation cannot respond to the great variety of atomic coordinates which evolves in time with typical atomic periods. In this sense, the classical thermodynamics is constructed under the paradigmatic notion of the all measurement are a process of coarse-graining. Thus, the measurement process effectively filters out redundant information, focusing solely on the variables relevant to the system's description. This redundant information are redundant only in the perspective of the classical thermodynamics [3].

On the other hands, in the context of the quantum mechanics, all information of the system are contained in a physical vector or more general in the density matrix operator ρ. Moreover, in the context of quantum mechanics, our ability to manipulate systems allows for a quantum description that is substantially more comprehensive than a classical description encompassing the entire physical system. This is particularly due to the intimate connection between the description of physical states and the eigenbasis (basis of the Hamiltonian) of the system's Hamiltonian operator [40].

Therefore, classical and quantum thermodynamics rely on very different paradigms. But the connection of this paradigms given us a perspective for the gauge notion in quantum thermodynamics. From this two distinct paradigms, motivate us to the introduce the concept of emergent redundancy in the quantum thermodynamics from the parallel to the measurement in classical thermodynamics.

In fact, since the physical states carries all physics information of the system we can see this states plays the same role as the potentials in the field theories, i.e. all relevant thermodynamics quantities are obtained by the physical states, more specific, the density matrix. Furthermore, in the same spirit of the classical thermodynamics, the same notion of coarse-graining is extended to the setting of quantum thermodynamics, implying that the all information are not necessary to the description of the relevant thermodynamics quantities [3].

This perspective given us the concept to the emergent gauge. In fact, the emergent gauge is associated to the redundancies in the thermodynamics theory, which not is fundamental as a gauge transformation in Electrodynamics or other field theories, but emerges from the nature of this description. Then, the emergent gauge not is fundamental, but he carries information about the symmetries and redundancies of the system in the thermodynamics context.

Having established the necessary background, we can now turn our attention to the construction of a framework for gauge-invariant quantum thermodynamics. First, we note the usual development presented in the section 2.2 are been considered from the start point to the this framework. Then, we will introduce a set of fundamental assumptions of this framework:

(i) All theory are defined over a finite $d-$dimension Hilbert space which us denote by $\mathcal{H}^d$.

(ii) The thermodynamics quantities are all treated as functionals of the density matrix $\rho \equiv \rho(t)$.

(iii) The gauge transformation are unitary linear transformation.

(iv) The gauge transformation preserves the energy (2.25) of the system.

The first assumption set all framework over a finite arbitrary d dimensional Hilbert space. In fact, this assumption is associated to a fact that a very large class of quantum systems which are interesting in quantum thermodynamics (qubits, heat machines, spins chains) are defined in a finite dimensional Hilbert space. A infinite dimensional extension can be considered, but mathematics problems can be emerges from this, like a divergences in operators.

The second hypothesis follows from the usual thermodynamics quantities presented in the section 2.2. Furthermore, the density matrix ρ is a physical state who carrier all physics information of the dynamics in this scenarios. Then, since all thermodynamics are treated as functionals of the density matrix we can evaluate all framework over the coarse-graining perspective for a quantum thermodynamics.

The last two assumptions are the particularly relevant from us. The item (iii) characterizes a gauge transformation and reduces all possible transformation to the unitary transformations which is natural choice since the linearity and unitary nature of quantum mechanics. Therefore, the assumptions (ii) and (iii) they characterize that the state ρ transformed by the gauge action must transform by:

$$\rho \to V_t \rho V_t^{\dagger}, \tag{3.22}$$

where V_t are an unitary transformation on $\mathcal{H}^d$ which is a candidate to a gauge transformation.

Por fim, a hipótese (iv) é necessária para eliminar a arbitrariedade na hipótese (iii) sob transformações unitárias. No entanto, há ainda um significado mais profundo que reside sob essa hipótese a qual alinha-se diretamente com a motivação física para nosso approach: Fixar as transformações de gauge desse modo garante a nós que conseguimos ter acesso a medições na base de energia.

Em particular, é essa hipótese então que estabelce o princípio de gauge do nosso formalismo. Nesse sentido, faz-se relevante estabelecermos esse resultado formalmente pela seguinte definição.

Definition 1. *(Principle of gauge energy invariance [3]) An unitary transformations* $V_t : \mathcal{H}^d \to \mathcal{H}^d$ *are admissible gauge transformation if it preserve the mean energy, independently of a particular state of the system i.e.*

$$\mathrm{U}[V_t \rho V_t^\dagger] = \mathrm{U}[\rho] \tag{3.23}$$

for all $\rho \in L^1\left(\mathcal{H}^d\right)$ *.*

That is, Eq. (3.23) restricts the unitary transformations to a specific subset of unitaries that are indeed admissible as gauge transformations for our theory. In particular, Eq. (3.23) thus establishes a thermodynamic equivalence class among quantum states with the same energy under the action of gauge transformations, even though these states may have very distinct informational meanings.

In this sense, we can say that the group formed by these transformations is emergent rather than fundamental. These transformations arise from our lack of control over the system, rather than from a fundamental redundancy in the system's description, as seen, for example, in Classical Electrodynamics discussed in Section 3.1. The limitation of control and informational access over quantum systems is quite natural. Indeed, if we aim to fully reconstruct the density matrix of an arbitrary system, a sufficiently large number of measurements in different bases would be required, which is often unfeasible, as described in the experiment in Ref. [78]. Even in a closed quantum system, quantum state tomography is prohibitive due to the dimension of the Hilbert space, allowing only energy measurements. Nevertheless, for the scenario of continuous quantum systems, not even point-like energy measurements are permitted, and energy measurements encompass a finite-sized energy window.

Having discussed the physics of the gauge principle, we can now proceed with the development starting from Def. 2 to obtain a general expression characterizing the admissible gauge transformations. Along this path, we present the following proposition.

Proposition 1. *Every unitary transformation* V_t *that satisfies the equality* (3.23) *of Definition 1 commutes with the Hamiltonian* $H \equiv H(t)$*, i.e.*

$$[V_t, H] = [V_t^\dagger, H] = 0. \tag{3.24}$$

Proof. If V_t satisfies the equality (3.23), then, from the definition of usual mean energy, we have the following development

$$\begin{aligned} \mathrm{U}[V_t\rho V_t^\dagger] = \mathrm{U}[\rho] &\implies \mathrm{Tr}\{V_t\rho V_t^\dagger H\} = \mathrm{Tr}\{\rho H\} \\ &\implies \mathrm{Tr}\{\rho V_t^\dagger H V_t\} = \mathrm{Tr}\{\rho H\} \\ &\implies \mathrm{Tr}\left\{\rho\left(V_t^\dagger H V_t - H\right)\right\} = 0 \end{aligned}$$

for all $\rho \in L^1(\mathcal{H}^d)$. Therefore, if we choose a ρ such that $\rho = |j\rangle\langle k|$ where $\{|n\rangle\}$ is a arbitrary orthonormal basis we have:

$$\begin{aligned} 0 &= \mathrm{Tr}\left\{\rho\left(V_t^\dagger H V_t - H\right)\right\} \\ &= \sum_n \langle n| \left[|j\rangle\langle k| \left(\sum_{l,m} a_{l,m} |l\rangle\langle m| - \sum_{q,r} b_{q,r} |q\rangle\langle r| \right)\right] |n\rangle \\ &= \sum_{n,l,m} a_{l,m}\delta_{n,j}\delta_{k,l}\delta_{m,n} - \sum_{n,q,r} b_{q,r}\delta_{n,j}\delta_{k,q}\delta_{r,n} \\ &= a_{k,j} - b_{k,j} \end{aligned}$$

therefore $a_{k,j} = b_{k,j}$ where $a_{k,j} = (V_t^\dagger H V_t)_{k,j}$ and $b_{k,j} = (H)_{k,j}$. Thus, all matrix elements are equal which implies:

$$V_t^\dagger H V_t - H = \vec{0} \implies HV_t - HV_t^\dagger = \vec{0} \implies [H, V_t] = \vec{0}$$

where $\vec{0}$ denotes the null vector. From this, the first equality are obtained. The second equality is directly, since H is hermitian operator we have

$$[V_t^\dagger, H]^\dagger = (V_t^\dagger H - HV_t^\dagger)^\dagger = (HV_t - V_t H) = [H, V_t]$$

therefore we obtain $[V_t, H] = [V_t^\dagger, H] = \vec{0}$, as wished. □

This result is interesting and will have significant consequences for future developments. In particular, the gauge transformation V_t acts on the Hamiltonian operator in a manner analogous to a unitary channel, as mentioned in Section 2.2. Furthermore, it is important to note regarding this result that, in the context of resource theory, we have thermal operations [79, 80], which are defined as quantum channels that commute with the total Hamiltonian, which is the sum of the Hamiltonians of the system, the reservoir, and the interaction between the system and the reservoir.

In our definition, the gauge transformation V_t does not equate to thermal operations, since the transformation V_t does not include the interaction of a thermal bath with the system in such a way that the thermal bath can be traced out from the system without affecting the determination of the gauge transformation V_t. However, the transformations V_t form a particular subset of thermal operations, where the bath-environment interaction is irrelevant [3].

Now, let us proceed with the construction of the gauge transformation in order to have a general expression for any given Hamiltonian. Since, by hypothesis, the gauge is unitary, it follows that the transformations V_t are representations of the unitary group of dimension d, i.e., $\mathcal{U}(d)$, the set of all linear transformations (matrices in this context) of order $d \times d$ that are unitary. In fact, the group $\mathcal{U}(d)$ will be the starting point for obtaining the group associated with our framework. In the sense of group representation theory, and since the Hamiltonian H is a Hermitian operator, we can write this as

$$H(t) = u_t \left(\bigoplus_{k=1}^{p} \lambda_k(t) \mathbb{1}_{n_t^k} \right) u_t^\dagger = u_t h(t) u_t^\dagger, \; h(t) \equiv \bigoplus_{k=1}^{p} \lambda_k(t) \mathbb{1}_{n_t^k} \tag{3.25}$$

where p is the number of its distinct eigenvalues, n_t^k is the multiplicity of each eigenvalue $\lambda_k(t)$, that is, n_t^k are the instantaneous degeneracy degrees such that $\sum_{k=1}^{p} n_t^k = d$ for each instant of time t and $\mathbb{1}_{n_t^k}$ is the identity matrix whose dimension is n_t^k. This implies that the degrees of degeneracy can change in time, but the constraint $\sum_{k=1}^{p} n_t^k = d$ is always satisfied in reason the Hamiltonian is hermitian operator for all values of t. In sequence, we can consider the construction to theory under this assumption with purpose to generalize the initially work proposed in [3].

Since the Hamiltonian can be decomposed as in (3.25), we can obtain a decomposition for the operators V_t such that equality (3.23) is satisfied. In particular, V_t can be decomposed into irreducible representations of some unitary group. In fact, we will show this result below.

Proposition 2. *Let $V_t : \mathcal{H}^d \to \mathcal{H}^d$ be a unitary transformation defined on the d-dimensional Hilbert space $\mathcal{H}^d$. Then, if $[V_t, H] = \vec{0}$, the transformation V_t can be written as:*

$$V_t = u_t \mathcal{V}_t u_t^\dagger, \quad \text{with} \;\; \mathcal{V}_t = \bigoplus_{k=1}^{p} v_t^k, \tag{3.26}$$

with $v_t^k \in \mathcal{U}(n_t^k)$ and $V_t \in \mathcal{U}(d)$, where the set $\mathcal{U}(d)$ represents the group of $d \times d$ unitary matrices.

Proof. Since the Hamiltonian operator H is hermitian follows from the decomposition of (3.25) and the equality (3.23) the following development:

$$\begin{aligned}
[H_t, V_t] = \vec{0} \quad &\Longrightarrow \quad u_t h u_t^\dagger V_t - V_t u_t h u_t^\dagger = \vec{0} \\
&\Longrightarrow \quad h u_t^\dagger V_t u_t - u_t^\dagger V_t u_t h = \vec{0} \\
&\Longrightarrow \quad \left[h, u_t^\dagger V_t u_t \right] = \vec{0} \\
&\Longrightarrow \quad [h, \mathcal{V}_t] = \vec{0}
\end{aligned}$$

where $\mathcal{V}_t = u_t^\dagger V_t u_t$. Expanding this commutator:

$$\begin{aligned}[h, \mathcal{V}_t] &= \left(\sum_l \lambda_l \left|l\right\rangle \left\langle l\right|\right)\left(\sum_{m,n} (\mathcal{V}_t)_{mn} \left|m\right\rangle \left\langle n\right|\right) - \left(\sum_{m,n} (\mathcal{V}_t)_{mn} \left|m\right\rangle \left\langle n\right|\right)\left(\sum_l \lambda_l \left|l\right\rangle \left\langle l\right|\right) \\ &= \sum_{m,n} \lambda_m (\mathcal{V}_t)_{mn} \left|m\right\rangle \left\langle n\right| - \sum_{m,n} \lambda_n (\mathcal{V}_t)_{mn} \left|m\right\rangle \left\langle n\right|.\end{aligned}$$

Now, for the element j, k we have:

$$\begin{aligned}\left\langle j\right| [h, \mathcal{V}_t] \left|k\right\rangle = \vec{0} \quad &\Longrightarrow \quad \sum_{m,n} \lambda_m (\mathcal{V}_t)_{mn} \delta_{j,m}\delta_{n,k} - \sum_{m,n} \lambda_n (\mathcal{V}_t)_{mn} \delta_{j,m}\delta_{n,k} = 0 \\ &\Longrightarrow \quad (\mathcal{V}_t)_{jk} \lambda_j - (\mathcal{V}_t)_{jk} \lambda_k = 0 \\ &\Longrightarrow \quad (\mathcal{V}_t)_{jk} (\lambda_j - \lambda_k) = 0.\end{aligned}$$

Therefore, if $\lambda_j \neq \lambda_k$ the last equality implies that $(\mathcal{V}_t)_{jk} = 0$ and, for symmetry $(\mathcal{V}_t)_{kj} = 0$ then the block jk is a simple diagonal block matrix which we denote by v_t^k, in addition $v_t^k \in \mathcal{U}(1)$ since V_t is unitary. On the other hands, if $\lambda_j = \lambda_k$ then the matrix element $(\mathcal{V}_t)_{jk}$ are arbitrary, real or complex and zero or nonzero. Additionally, the matrix block j, k are non diagonal which implies that $v_t^k \in \mathcal{U}(n_t^k > 1)$ which n_t^k is degree of degenerated of each eigenvalue.

Consequently, the matrix $\mathcal{V}_t$ can be decomposed into a direct sum of unitary matrices v_t^k, each associated with the group $\mathcal{U}(n_t^k \geq 1)$, as follows:

$$\mathcal{V}_t = \bigoplus_{k=1}^{p} v_t^k \implies u_t^\dagger V_t u_t = \bigoplus_{k=1}^{p} v_t^k \implies V_t = u_t \bigoplus_{k=1}^{p} v_t^k u_t^\dagger,$$

and thus, we have arrived at the desired result. □

The result of Proposition 2 is associated with the obtaining of a set of irreducible representations v_t^k of the unitary group $\mathcal{U}(n_t^k)$; in particular, each unitary representation is associated with a Hilbert subspace of $\mathcal{H}^d$ that we denote by $\mathcal{H}_k$. In effect, the matrix $\mathcal{V}_t$ is then a block diagonal matrix, with each v_t^k being one of its elements.

With the general expression for the gauge transformation V_t at hand, we can then define the gauge group for quantum thermodynamics. In fact, this gauge group is formally defined by:

Definition 2. *(Thermodynamic group) Let $H \equiv H(t)$ be a time dependent Hamiltonian operator defined on a d-dimensional Hilbert space $\mathcal{H}^d$ and u_t be defined as in Eq. (3.25). Then, the thermodynamics gauge group is defined as the following set of transformations*

$$\mathcal{T}_H = \left\{ V_t \in \mathcal{U}(d) |\, [V_t, H] = 0, V_t = u_t \left(\bigoplus_{k=1}^{p} v_t^k\right) u_t^\dagger \right\} \tag{3.27}$$

where $v_t^k \in \mathcal{U}(n_t^k) \subset \mathcal{U}(d)$ *and* $\Gamma = \{n_t^k\}_{k=1,\dots,p}$ *is the set of labels of the degeneracies of the eigenvalues of* H *at time* t*.*

The thermodynamic or gauge group is associated to each instant $t \in (t-\epsilon, t+\epsilon)$ with arbitrary $\epsilon > 0$. Therefore, all gauge transformations are defined in instantaneous form with is related to changes in the degeneracy set Γ.

From the topological point of view the thermodynamic gauge group can be analyzed by the by the introduction to isomorphic group $\mathcal{G}_{\mathrm{T}}$ with is associated to each matrix $\mathcal{V}_t$ in (3.26). The following proposition, establishes the group $\mathcal{G}_{\mathrm{T}}$:

Proposition 3. *($\mathcal{G}_{\mathrm{T}}$-group) The emergent gauge group is isomorphic to the gauge group $\mathcal{G}_{\mathrm{T}}$ defined by:*

$$\mathcal{G}_{\mathrm{T}} = \mathcal{U}(n_t^1) \times \mathcal{U}(n_t^2) \times \dots \times \mathcal{U}(n_t^k), \tag{3.28}$$

for each instant t, where $\times$ denote the Cartesian product.

Proof. Trivial. □

Since the group $\mathcal{G}_{\mathrm{T}}$ is isomorphic to the group E_H, we will sometimes refer to $\mathcal{G}_{\mathrm{T}}$ as the emergent gauge group or simply gauge group.

The gauge group is directly associated to the decomposition of the gauge V_t in him irreducible representations v_t^k given in (3.26) and consequently to the subgroups $\mathcal{U}(n_t^k)$ of $\mathcal{U}(d)$. In fact, this groups is construct by a finite Cartesian product of the compact Lie subgroups, therefore, $\mathcal{G}_{\mathrm{T}}$ is also compact Lie group, whose Lie algebra we denote by $\mathfrak{g}_{\mathrm{T}}$. In special, the dimension of the Lie algebra of the gauge group is specially interesting to this framework, firstly this Lie Algebra is associated to the Hilbert space $\mathcal{H}^d$ which is decomposed in the following direct sum: $\mathcal{H}^d = \bigoplus_{k=1}^{p} \mathcal{H}_k$. This isomorphism is represented below in Fig 3.1.

From the Proposition 2 we can see that the dimension of Lie algebra of $\mathcal{G}_{\mathrm{T}}$ is determined by the degeneracies in the Hamiltonian spectrum. Specially, in the case of the Hamiltonian is non-degenerated each v_t^k matrix is a simple element of unitary group $\mathcal{U}(1)$, i.e.v_t^k is complex a number which is completely identified by one parameter. On the other hands, if each $\lambda_k(t)$ is a degenerated eigenvalue, for example double degenerated, the matrix v_t^k is a unitary 2×2 matrix and $v_t^k \in \mathcal{U}(2)$ which elements can be are nonzero.

Then, the dimension of Lie algebra of the $\mathcal{G}_{\mathrm{T}}$ group in these cases are $\dim\{\mathfrak{g}_{\mathrm{T}}\} = \dim\{\mathcal{U}(1)\} + \dots + \dim\{\mathcal{U}(1)\} = d$ and $\dim\{\mathfrak{g}_{\mathrm{T}}\} = \dim\{\mathcal{U}(2)\} + \dots + \dim \mathcal{U}(2) = 4d$. This reveals the following result: degeneracies in the Hamiltonian spectrum implies in more redundancies in the system which are related to the dimension of the Lie algebra of the gauge group. From the topological

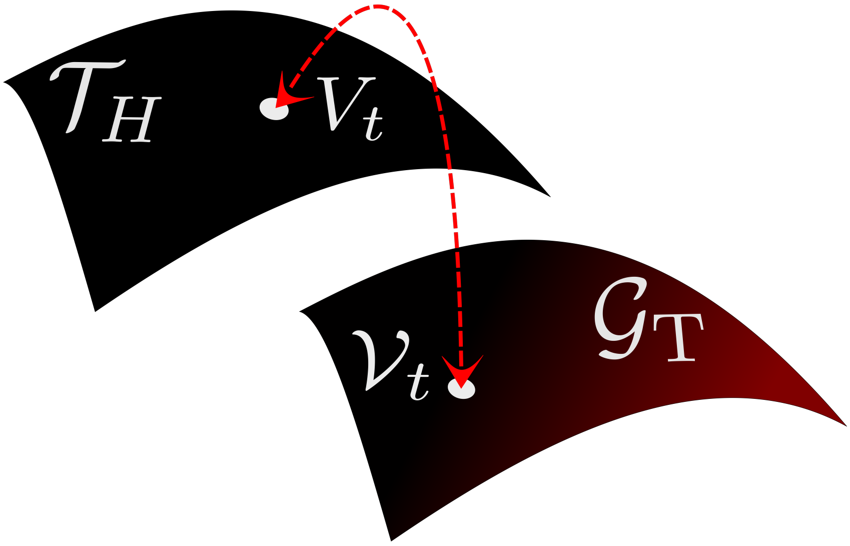

FIGURE 3.1: Schematic representation of the isomorphism between the differential manifold of the thermodynamic group $\mathcal{T}_H$ and the gauge group $\mathcal{G}_{\mathrm{T}}$. This isomorphism allows us to identify the general structure of the Hamiltonian symmetry unitaries V_t as a direct sum of unitaries v_t^k associated with each Hilbert subspace $\mathcal{H}_k$.

perspective, gauge group, which is a Lie group, defines a manifold which dimension is given by

$$\dim\{\mathfrak{g}_{\mathrm{T}}\} = \sum_{k=1}^{p} \dim\{\mathcal{U}(n_t^k)\} = \sum_{k=1}^{p} (n_t^k)^2, \tag{3.29}$$

where the maximum dimension of this Lie algebra is obtained when $n_t^k = d$, therefore in this case $\dim\{\mathfrak{g}_{\mathrm{T}}\} = d^2$, which occurs when the Hamiltonian spectrum is completely degenerated, i.e. all eigenvalues are equal.

Since the degeneracies of the Hamiltonian can be changed in time, the dimension of the manifold of the gauge group changes in time. Consequently, for a time-dependent Hamiltonian evolving under a specified protocol, the gauge group continuously adapts to encompass submanifolds within the maximal manifold defined by H, specifically when its spectrum attains the maximum possible degeneracy. In fact, for a given Hamiltonian the case when all eigenvalues are equal is impossible, however, there exists a maximum number of degeneracies that can occur, so for a given Hamiltonian the maximum dimension of the Lie algebra of the gauge group is

$$\max\left[\dim\{\mathfrak{g}_{\mathrm{T}}\}\right] = \max_{t\in\mathbb{R}} \left[\sum_{k=1}^{p} \dim \mathcal{U}(n_t^k)\right] \leq d^2. \tag{3.30}$$

This construct establishes the mathematical formalism from the thermodynamics or emergent gauge group. Indeed, so far we have only constructed the notion of gauge group and gauge transformation for thermodynamics, but we have not yet introduced any aspects related to the description of quantum thermodynamics. In this sense, in the following section we will introduce the notion of functionals and invariant spaces, which is where we will construct new quantities of interest for quantum thermodynamics.

3.3 Gauge theory of $\mathcal{G}_{\mathrm{T}}$-group

The thermodynamics group is the fundamental element in the formalism we are establishing. However, the notion of invariance introduced in Definition 1 should not be restricted simply to the unitary transformations V_t that we constructed in Proposition 2. In fact, the main physical quantities in the context of thermodynamics, such as work for example, are not invariant under the gauge transformation V_t, indeed, note that:

$$\begin{aligned}
W_u[V_t\rho V_t^\dagger] &= \int_0^\tau dt\,\mathrm{Tr}\left\{V_t\rho V_t^\dagger\frac{dH}{dt}\right\}\\
&= \int_0^\tau dt\,\mathrm{Tr}\left\{\rho\left[\frac{d(V_t^\dagger HV_t)}{dt}-\frac{dV_t^\dagger}{dt}HV_t-V_t^\dagger H\frac{dV_t}{dt}\right]\right\}\\
&= \int_0^\tau dt\,\mathrm{Tr}\left\{\rho\frac{dH}{dt}-\left[-H\rho V_t^\dagger\frac{dV_t}{dt}+\rho HV_t^\dagger\frac{dV_t}{dt}\right]\right\}\\
&= \int_0^\tau dt\,\mathrm{Tr}\left\{\rho\frac{dH}{dt}+[\rho,H]V_t^\dagger\frac{dV_t}{dt}\right\}\\
&= W_u\left[\rho\right]+\int_0^\tau dt\,\mathrm{Tr}\left\{[\rho,H]V_t^\dagger\frac{dV_t}{dt}\right\}.
\end{aligned}$$

Consequently, we have that $W_u[V_t\rho V_t^\dagger]\neq W_u[\rho]$ since the equality $[\rho,H]=0$ does not always hold. In particular, this follows from the fact that certain functionals of the density matrix operator are not necessarily invariant under unitary transformations. In this sense, we will construct a notion such that functionals, especially the functionals relevant in the context of thermodynamics, are invariant under the gauge transformation V_t.

From this perspective, the subscript u, introduced in all thermodynamics quantities in the Section 2.2, plays a important to denotes the usual thermodynamics quantities since further we going to introduce a new analogous notions (heat and work) which are invariant counterpart with respect to the emergent gauge group.

To this end, we will construct the notions of invariant Hilbert spaces in the context of the thermodynamic gauge group. In effect, note that the gauge group, defined by the isomorphism (3.28), is the product of different unitary groups, all of which are compact Lie groups [81]. Therefore, it follows that the gauge group is also a compact Lie group, and thus there exists a unique normalized, left and right invariant measure [81] associated with the group $\mathcal{G}_{\mathrm{T}}$, which we denote by:

$$d\mathcal{G}_{\mathrm{T}}=d\mu\left[\mathcal{U}(n_t^1)\right]\times d\mu\left[\mathcal{U}(n_t^2)\right]\times\ldots\times d\mu\left[\mathcal{U}(n_t^p)\right] \tag{3.31}$$

where $d\mu\left[\mathcal{U}(n_t^k)\right]$ are the Haar measure associated to unitary group $\mathcal{U}(n_t^k)$ for all values of k, and $d\mathcal{G}_{\mathrm{T}}$ is a multidimensional Haar measure. In apppendix B.2 we formally present the Definition of Haar measure for compact Lie groups and some properties.

Since this measure is defined with respect to time, and as the set of degeneracies of the Hamiltonian may change, it is necessary to introduce a general Haar measure that preserves the maximal measure element obtained when the system has d degeneracies. In effect, the Haar measure associated with the group $\mathcal{U}(d)$ is then decomposed into:

$$d\mu[\mathcal{U}(d)] = d\mathcal{G}_{\mathrm{T}} \cdot d\mathcal{G}_{\mathrm{T}}^{c}, \tag{3.32}$$

where $d\mathcal{G}_{\mathrm{T}}$ is defined in (3.31) and $d\mathcal{G}_{\mathrm{T}}^{c}$ denotes the complementary measure with respect to the Haar measure of the gauge group defined in Eq. (3.31).

In effect, both $d\mathcal{G}_{\mathrm{T}}$ and $d\mathcal{G}_{\mathrm{T}}^{c}$ are normalized Haar measures. However, we must introduce $d\mathcal{G}_{\mathrm{T}}^{c}$ to ensure that the dimensionality of the measure is always guaranteed; in this sense, we complete the dimensionality until we achieve the maximum possible dimensionality, equivalently, the maximum configuration of degeneracies. Indeed, this technical aspect allows us to modify the measure $d\mathcal{G}_{\mathrm{T}}$ across any interval associated with the parameter t since the complementary measure ensures the preservation of dimensionality. Nevertheless, note that the complementary measure is merely a mathematical artifact introduced to ensure the consistency of the modification of the gauge group's measure, such that it is only relevant to consider the integration with respect to the induced measure of the thermodynamic gauge group.

With this in mind, we can then define the notion of invariant quantities with respect to the gauge group, using group averaging techniques. This leads to the definition of gauge-invariant quantities or physical quantities as follows:

Definition 3. *(Gauge-invariant quantities). Given functional (linear or not) $F[\rho]$ which are not invariant over unitary transformation, its counterpart invariant with respect to the thermodynamic gauge group is*

$$F_{inv}[\rho] = \int d\mathcal{G}_{\mathrm{T}} F\left[V_t \rho V_t^{\dagger}\right], \tag{3.33}$$

and if $F[\rho]$ is invariant over unitary transformation, its counterpart invariant with respect to the emergent gauge group is:

$$F_{inv}[\rho] = F\left[\mathrm{D}(\rho)\right], \tag{3.34}$$

where D is a linear operator in $\mathcal{H}^d$ defined by $\mathrm{D}(\cdot) \equiv \int d\mathcal{G}_{\mathrm{T}} V_t (\cdot) V_t^{\dagger}$, V_t is given in (3.26) and $d\mathcal{G}_{\mathrm{T}}$ is the multi dimensional Haar measure on the group $\mathcal{G}_{\mathrm{T}}$ defined in (3.31).

Definition 3 establishes the notion of invariant quantities. In particular, in the context of the first law of thermodynamics, we are interested in studying the functionals $W_u[\rho]$ and $Q_u[\rho]$, both of which are linear and non-invariant under unitary transformations, thus their invariant counterparts are given by Eq. (3.33). In special, the subset of all linear functionals obtained by (3.33) forms a subspace of the dual space $\mathcal{H}^{d'}$ of the Hilbert space $\mathcal{H}^d$.

Furthermore, with Definition 3, we obtain the key elements for our formulation of thermodynamics as a gauge theory. Schematically, these elements are represented in Figure 3.2 below.

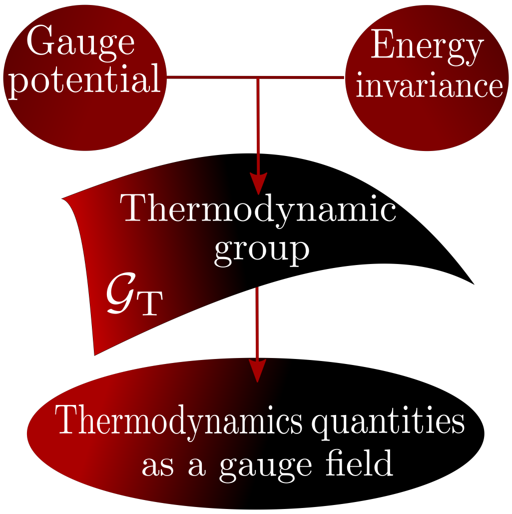

FIGURE 3.2: $\mathcal{G}_\mathrm{T}$-thermodynamics. The density operator acts as a gauge potential, with the Hamiltonian's internal symmetries constrained by average energy invariance. This defines the thermodynamic group $\mathcal{T}_H$, formed by all unitaries V_t commuting with H. The Lie group $\mathcal{G}_\mathrm{T}$, isomorphic to $\mathcal{T}_H$ is built and connect to the irreps of each k-eigenspace of H, inducing the Haar measure $\mathrm{d}\mu\,\mathcal{G}_\mathrm{T}$. Physical quantities, treated as a gauge fields, emerges through Haar averaging over $\mathcal{G}_\mathrm{T}$ group.

The Haar integral which appears in the Definition 3 can be interpreted by the averaging of the integrand over all elements in the group and this implies that this integral can remove all redundancies established by the group whose induced the Haar measure [82]. Here, the discussion of dimension of Lie algebra of the gauge group returns, in special we can see that the contributed of the degeneracies can increase the dimension of the Lie algebra of the gauge group and, conversely, the integral is evaluated over the more elements with respect to the non-degenerate case.

Another important aspect is associated to the two definitions of gauge invariant quantities in 3. In fact, the objective of gauge transformation employed here is associated to capture and wash away redundancies information in quantum states, whose carriers of quantum information of the physical system. However, the assumption of the gauge is a linear and unitary transformation any physical quantities invariant under unitary transformation is immediately invariant over Haar integral, therefore if we assume the unique definition in Eq. (3.33) we have $F_{inv}[\rho] = F[\rho]$ and no redundancy information has been eliminated. Therefore, the definition Eq. (3.33) is not enough to define the invariant quantities, in this sense we extend the initial propose in [3] introducing the second notion in Eq. (3.34). Specially, for functionals invariant under the unitary transformation the linear operator D eliminate the redundancy information in density operator and apply this in functional F.

3.3.1 Quantum twirling operator

Definition 3 introduces the linear operator D. Indeed, this operator is sufficiently important in our context as it guarantees the elimination of redundancies in the state described by the density matrix. Furthermore, we can connect it to an important class of operators: the quantum twirling operators.

Moreover, we can formally present this

$$\begin{aligned} D: L^1(\mathcal{H}^d) &\rightarrow L^1(\mathcal{H}^d)_{inv} \subset L^1(\mathcal{H}^d) \\ \rho &\rightarrow D(\rho) = u_t \left(\int d\mathcal{G}_{\mathrm{T}} \mathcal{V}_t \rho^E \mathcal{V}_t^\dagger \right) u_t^\dagger, \end{aligned} \tag{3.35}$$

where $\rho^E = u_t^\dagger \rho u_t$ correspond the density matrix in energy eigenbasis (denoted by superscript E). The subspace $L^1(\mathcal{H}^d)_{inv}$ of the $L^1(\mathcal{H}^d)$ is the Hilbert space of the invariant states with respect to the Haar average.

Particularly, from the perspective of information theory, specially, from the quantum information theory, the operator $D(\rho)$ is a quantum channel [41, 83]. In this sense, we are motivate to define the following auxiliary operator:

$$\begin{aligned} \Lambda_{\mathcal{G}_{\mathrm{T}}}: L^1(\mathcal{H}^d) &\rightarrow L^1(\mathcal{H}^d)_{inv} \subset L^1(\mathcal{H}^d) \\ X(t) \in L^1(\mathcal{H}^d) &\rightarrow \Lambda_{\mathcal{G}_{\mathrm{T}}}[X(t)] = \int d\mathcal{G}_{\mathrm{T}} \mathcal{V}_t X(t) \mathcal{V}_t^\dagger \end{aligned} \tag{3.36}$$

for some operator $X(t)$, which are called quantum Twirling operator [83, 84]. In fact, the Twirling operator (3.36), or superoperator, appears in the context of the unitary $k-$designer [84–86] associated a noisy quantum channel. Particularly, the integral in (3.36) can be evaluated analytically for any operator X, since X is Haar integrable and the Haar measure is known, specially by the general Haar measure induced by the gauge group (3.31) we have:

$$X_{dd}(t) \equiv \Lambda_{\mathcal{G}_{\mathrm{T}}}[X(t)] = \int d\mathcal{G}_{\mathrm{T}} \mathcal{V}_t X(t) \mathcal{V}_t^\dagger = \bigoplus_{k=1}^{p \leq d} \frac{\mathrm{Tr}\{X_{n_t^k}(t)\}}{n_t^k} \mathbb{1}_{n_t^k} \tag{3.37}$$

where $X_{n_t^k} = \Pi_{n_t^k} X \Pi_{n_t^k}$ with $\Pi_{n_t^k}$ the projector associated to the each subspace spanned for the eigenvectors related to the kth eigenenergy.

The result obtained in Eq. (3.37) is known in the literature [87]. Moreover, its derivation requires the use of several technical details that involve the use of group averaging techniques and results from group representation theory. In this sense, the interested reader can refer to Appendix B, more specifically in section B.2.

With equality in Eq. (3.37), we can obtain some properties associated with the quantum twirling operator. In particular, we will show that it is a unital quantum channel; more details can be found in Appendix B.2. That is, we will demonstrate that the quantum twirling operator is a completely positive trace-preserving (CPTP) map and that $\Lambda_{\mathcal{G}_{\mathrm{T}}}[\mathbb{1}] = \mathbb{1}$. In this sense, we have:

- Since the quantum twirling operator is given by (3.37), it follows that for any density matrix ρ, we will have:

  $$\Lambda_{\mathcal{G}_{\mathrm{T}}}[\rho(t)] = \bigoplus_{k=1}^{p\leq d} \frac{\mathrm{Tr}\left\{\rho_{n_t^k}(t)\right\}}{n_t^k}\mathbb{1}_{n_t^k}. \tag{3.38}$$

  In other words, the matrix resulting from the quantum twirling operator is a diagonal matrix whose diagonal elements are formed by sums of the diagonal elements of the matrix ρ. Therefore, all of these are positive, and thus the map $\Lambda_{\mathcal{G}_{\mathrm{T}}}$ preserves the positivity of the density operator.

- This operator preservers the trace. Indeed:

  $$\mathrm{Tr}\left\{\Lambda_{\mathcal{G}_{\mathrm{T}}}[\rho]\right\} = \mathrm{Tr}\left\{\int d\mathcal{G}_{\mathrm{T}}\mathcal{V}_t\rho\mathcal{V}_t^\dagger\right\} = \int d\mathcal{G}_{\mathrm{T}}\,\mathrm{Tr}\left\{\mathcal{V}_t\rho\mathcal{V}_t^\dagger\right\} = \mathrm{Tr}\{\rho\}. \tag{3.39}$$

  Since the cyclicity of the trace gives us $\mathrm{Tr}\left\{\mathcal{V}_t\rho\mathcal{V}_t^\dagger\right\} = \mathrm{Tr}\left\{\rho\mathcal{V}_t^\dagger\mathcal{V}_t\right\} = \mathrm{Tr}\{\rho\}$, because the matrices $\mathcal{V}_t$ are unitary. Therefore, the map $\Lambda_{\mathcal{G}_{\mathrm{T}}}$ preserves the trace.

- Finally, note that for the identity operator we have:

  $$\Lambda_{\mathcal{G}_{\mathrm{T}}}[\mathbb{1}] = \int d\mathcal{G}_{\mathrm{T}}\mathcal{V}_t\mathbb{1}\mathcal{V}_t^\dagger = \int d\mathcal{G}_{\mathrm{T}}\mathcal{V}_t\mathcal{V}_t^\dagger = \int d\mathcal{G}_{\mathrm{T}}\mathbb{1} = \mathbb{1} \tag{3.40}$$

  therefore, the quantum twirling operator is a unital quantum channel.

In fact, the property that the quantum twirling operator is a unital quantum channel will be extremely useful for proving some properties of functionals such as the entropy that we will define in Chapter 4.

Certainly, we can introduce a twirling operator that allows our linear operator D to be written as:

$$\mathrm{D}[\rho(t)] = u_t\left(\int d\mathcal{G}_{\mathrm{T}}\mathcal{V}_t\rho^E(t)\mathcal{V}_t^\dagger\right)u_t^\dagger = u_t\Lambda_{\mathcal{G}_{\mathrm{T}}}[\rho^E(t)]u_t^\dagger = u_t\rho_{dd}^E(t)u_t^\dagger \tag{3.41}$$

where

$$\rho^E_{dd}(t) = \Lambda_{\mathcal{G}_\mathrm{T}}[\rho^E(t)] = \bigoplus_{k=1}^{p\leq d} \frac{\mathrm{Tr}\{\rho^E_{n^k_t}(t)\}}{n^k_t} \mathbb{1}_{n^k_t}, \quad \rho_{n^k_t} = \Pi_{n^k_t}\rho^E\Pi_{n^k_t}. \tag{3.42}$$

Then, in the case of the functionals, which are invariant under the unitary transformations, they functionals can be writen explicity in terms of the Twirling operator:

$$F_{inv}[\rho(t)] = F[D(\rho)] = F\left[u_t\Lambda_{\mathcal{G}_\mathrm{T}}[\rho^E(t)]u_t^\dagger\right] = F\left[\Lambda_{\mathcal{G}_\mathrm{T}}[\rho^E(t)]\right] = F[\rho^E_{dd}(t)] \tag{3.43}$$

since the u_t is a unitary transformation. In the context of Haar integral, $F_{inv}[\rho]$ is associated a functional evaluated using the averaging of the density matrix in energy eigenbasis over all elements in gauge group, i.e. the redundancy information has been eliminated in energy eigenbasis.

3.3.2 Invariant states

In effect, the property that characterizes $\Lambda_{\mathcal{G}_\mathrm{T}}$ as a unital quantum channel, i.e., Eq. (3.40), shows us that the state $\rho = \dfrac{\mathbb{1}}{d}$ is a fixed point of the operator $\Lambda_{\mathcal{G}_\mathrm{T}}$. In fact, just as this operator, there may be other states that are fixed points of $\Lambda_{\mathcal{G}_\mathrm{T}}$. In summary, these states are those that are naturally invariant under the thermodynamic gauge group. Note that in this case, the discussion is distinct from that which we used to introduce the second definition of invariant quantities in the previous section; here, we have states that are invariant not under unitary transformations but rather by the gauge transformation defined by Eq. (3.26).

So, let us now define the set of these invariant states as:

Definition 4. *(Invariant States) The set of invariants states over the gauge group is defined by:*

$$E_{inv} = \left\{\rho \in \mathcal{L}^1(\mathcal{H}^d) |\, \mathrm{D}[\rho] = \rho\right\}. \tag{3.44}$$

Note that the equality $\mathrm{D}[\rho] = \rho$ can be rewritten in terms of the Twirling operator through the following development:

$$\mathrm{D}[\rho] = \rho \quad \Longrightarrow \quad u_t\Lambda_{\mathcal{G}_\mathrm{T}}[\rho^E(t)]u_t^\dagger = \rho \tag{3.45}$$

$$\Longrightarrow \quad \Lambda_{\mathcal{G}_\mathrm{T}}[\rho^E(t)] = \rho^E(t). \tag{3.46}$$

Certainly, invariant states represent a peculiar and interesting subset of states that emerge from the mathematical formulation of this formalism. With this in mind, we will explore what types of states ρ belong to the set E_{inv}.

First, we will consider the case where the invariance arises from the Haar average. Thus, from Eq. (3.37) for the operator ρ^E, we must have:

$$\Lambda_{\mathcal{G}_{\mathrm{T}}}[\rho^E] = \rho^E \implies \frac{\mathrm{Tr}\{\rho_{n_t^k}(t)\}}{n_t^k} = \rho^E_{mm} \tag{3.47}$$

for all the n_t^k labels of m, that is, $\{m_1, m_2, ..., m_k\}$ associated with the subspace $\mathcal{H}_k$, it follows immediately that ρ^E must necessarily be diagonal. Furthermore, Eq. (3.47) provides us with a linear system of n_t^k equations, which are of the form:

$$\begin{cases} (1-n_t^k)\rho^E_{m_1m_1} + \sum_{l=2}^{k} \rho^E_{m_lm_l} = 0 \\ \rho_{m_1m_1} + (1-n_t^k)\rho_{m_2m_2} + \sum_{l=3}^{k} \rho^E_{m_lm_l} = 0 \\ \vdots \\ \sum_{l=1}^{k-1} \rho^E_{m_lm_l} + (1-n_t^k)\rho^E_{m_km_k} = 0 \end{cases} . \tag{3.48}$$

This set of n_t^k equations is linearly dependent and provides infinitely many solutions. However, the solutions of the system are fixed by a constraint among all the elements of the density operator. In fact, by subtracting each equation pairwise, it is possible to obtain that:

$$\rho^E_{m_1,m_1} = \rho^E_{m_2,m_2} = \ldots = \rho^E_{m_k,m_k} \tag{3.49}$$

In other words, we obtain that a given block is invariant if all the elements of the density matrix associated with that subspace are equal; consequently, this is the condition that each block is maximally mixed in its subspace. In fact, this further implies that if ρ^E is a state invariant under the Haar average, we can associate this state as being one obtained from a Twirling with the Haar measure defined by Eq. (3.31). Consequently, a state will be invariant with respect to the average if all its blocks are invariant, i.e., maximally mixed with respect to each subspace $\mathcal{H}_k$. Certainly, this result is already expected and well-known in the context of quantum computing and resource theories [41, 83, 88].

On the other hand, the coarse-graining defined by the Haar measure in Eq. (3.31) allows another type of state invariance to emerge. Certainly, since the gauge is not just any unitary transformation, its commutativity property allows other states to be invariant. In this context, for example, the Gibbs states:

$$\rho_G = \frac{e^{-\beta H}}{Z} \tag{3.50}$$

where β is the inverse of the temperature and Z is a partition function given by $Z = \mathrm{Tr}\left\{e^{-\beta H}\right\}$.

Effectively, these states are naturally invariant since we can treat them as functions of the Hamiltonian, and consequently, this state commutes with the matrices of the gauge group, thus the state is invariant under Haar averages. In summary, all states with explicit dependence on the Hamiltonian are invariant states.

Finally, it is also worth mentioning the particular case where there are no degeneracies in the system. In this case, the induced measure of the gauge group is given by a product of Haar measures of the group $\mathcal{U}(1)$, that is:

$$d\mathcal{G}_{\mathrm{T}} = \prod_{k=1}^{d} d\mu[\mathcal{U}(1)]. \tag{3.51}$$

Consequently, the Haar average of any density operator reduces from Eq (3.42) to:

$$\bigoplus_{k=1}^{d} \frac{\mathrm{Tr}\{\rho^{E} \left|k\right\rangle \left\langle k\right|\}}{n_t^k} = \rho_{diag}^{E} \tag{3.52}$$

where $n_t^k = 1$ for all k. That is, the Haar average reduces to the diagonal part of the energy basis density matrix. Consequently, the criterion for invariance under the Haar average reduces to the imposition that ρ^E be diagonal.

In summary, this construction leads us to formalize the following result.

Proposition 4. *Consider the operator $\rho \in \mathcal{L}^1(\mathcal{H}^d)$, then ρ belongs to the set E_{inv} if and only if it is diagonal in the energy basis and satisfies at least one of the following properties:*

(i) Each block n_t^k of the operator ρ_{dd}^E is maximally mixed in its subspace $\mathcal{H}_k$,

(ii) The state ρ is associated with some statistical ensemble.

3.4 Some considerations of the gauge approach

With Sections 3.2 and 3.3, we have constructed the fundamental notions of the gauge formalism for quantum thermodynamics. However, there are some important considerations we must address before proceeding with the work.

First, in consequence the constraint established by Definition 1, there is a natural class of quantities which are gauge-invariant by construction. These are all quantities solely defined on the equilibrium manifold. More general, they quantities which solely depend on the Hamiltonian, e.g., the microcanonical state are preserved [3].

The first point is associated to the existence of two transformations here. The first set of transformation are the unitary transformations that are the elements on gauge group $\mathcal{G}_{\mathrm{T}}$, which describes the symmetry transformations on the system and not dynamical processes. These transformations their role is to identify the set of states, for each instant of time, that cannot be distinguished by measuring thermodynamic variables. The other set of transformations are associated to physical process, which can be any complete positive and trace preserving map, including adiabatic (reversible) transformations, quenches and others. These are the ones governing the time evolution of the physical system, which implies our theory applies to both equilibrium and non-equilibrium transformations [3].

Finally, there is a crucial point for us to discuss: the choice of the invariance principle. In summary, the entire development done in Sections 3.2 and 3.3 is based on the hypotheses of the theory mentioned at the beginning of Section 3.2. Indeed, the non-triviality of the theory is ensured by hypothesis (iv), which establishes a gauge invariance criterion and determines the entire subsequent construction of the theory.

However, hypothesis (iv) admits a generalization, at least from the mathematical perspective of the theory. Indeed, instead of characterizing the theory by fixing the principle based on energy invariance, we can state it more generally for any observable $\mathcal{O}$ as follows:

Definition 5. *(Gauge observable invariance) An unitary transformations $V_t : \mathcal{H}^d \to \mathcal{H}^d$ are admissible gauge transformation if the preserve the expected value of a fixed observable $\mathcal{O}$, independently of a particular state of the system i.e.*

$$\langle \mathcal{O} \rangle_\rho = \langle \mathcal{O} \rangle_{V_t \rho V_t^\dagger} \iff \mathrm{Tr}\left\{\mathcal{O}\rho\right\} = \mathrm{Tr}\left\{V_t \rho V_t^\dagger \mathcal{O}\right\} \tag{3.53}$$

for all $\rho \in L^1\left(\mathcal{H}^d\right)$.

Indeed, the choice $\mathcal{O} = H$ retrieves Definition 1 and consequently all the results obtained in Sections 3.2 and 3.3. However, the generalized version of the invariance principle leads to analogous results, which are:

- The comutativity relation:
$$[V_t, \mathcal{O}] = [V_t^\dagger, \mathcal{O}] = \vec{0}.$$
- The decomposition of the observable $\mathcal{O}$:
$$\mathcal{O} = u_t^O O(t) u_t^{O\dagger}, \quad O(t) = \bigoplus_{k=1}^{p \leq d} \lambda_{\mathcal{O}}(t) \mathbb{1}_{n_t^k}$$
  where u_t^O is the matrix that diagonalizes the observable $\mathcal{O}$, and n_t^k is the degeneracy of each eigenvalue of the observable $\mathcal{O}$.

- The general form of the gauge transformation:

  $$V_t = u_t^O \mathcal{V}_t u_t^{O\dagger},\ \mathcal{V}_t = \bigoplus_{k=1}^{p\leq d} v_t^k$$

  with $v_t^k \in \mathcal{U}(n_t^k)$.

- The gauge group is defined by:

  $$\mathcal{T}_{\mathcal{O}} = \left\{ V_t \in \mathcal{U}(d) |\, [V_t, \mathcal{O}] = 0, V_t = u_t^O \left(\bigoplus_{k=1}^{p} v_t^k \right) u_t^{O\dagger} \right\}. \tag{3.54}$$

- The Haar measure induced from the gauge group:

  $$d\mathcal{G}_{\mathrm{T}} = d\mu \left[\mathcal{U}(n_t^1)\right] \times d\mu \left[\mathcal{U}(n_t^2)\right] \times ... \times d\mu \left[\mathcal{U}(n_t^p)\right]. \tag{3.55}$$

  where $p \leq d$.

In other words, the entire theory is developed analogously. However, the gauge group is modified such that the topological structure of the Haar measure is associated with the degeneracy degrees of the observable $\mathcal{O}$. Consequently, the manifold defined by the gauge group may be distinct from that of the Hamiltonian operator.

Furthermore, certain complications arise from this generalized choice. Indeed, we will see in the following sections that the choice of the invariance principle over the Hamiltonian leads to various simplifications in usual expressions within the thermodynamics context, particularly showing certain consistencies with existing literature results, thus favoring the choice of this principle.

Nonetheless, it is important to consider that this generalization arises from a mathematical perspective on the theory. In this sense, the initial choice of the invariance principle over energy introduced in Ref. [3] brings a physical significance that relates to the relevance of the energy basis in the context of quantum thermodynamics. Since the coarse-graining introduced by the definition of invariant quantities is then based on the manifold of the gauge group associated with the Hamiltonian, it consequently relates to the energy basis.

Chapter 4

Laws of quantum thermodynamics in gauge approach

In this chapter, we study the Laws of quantum thermodynamics over the perspective of the gauge-invariant approach establishes in the last chapter.

Accordingly, we structure the chapter into three sections. In the first, we present a novel result within the gauge formalism: the derivation of an explicit dynamical equation governing the density operator invariant under the thermodynamic group. This result provides a consistent and systematic physical interpretation for the thermodynamic quantities that will be developed in the subsequent sections.

The second section is dedicated to obtaining the concepts of heat and work that have already been derived for continuous protocols in the work of Céleri and Rudnicki [3]. Thus, we derive in detail all the expressions obtained in their work and discuss the physical aspects associated with the invariant quantities of heat and work, bringing a new perspective on their interpretations.

In the following section, we develop the notion of entropy in the context of gauge-invariant quantum thermodynamics and discuss its properties and relationships with other entropies, such as observational and diagonal entropy. Here, all results and discussions are based on original findings from this work, which are grounded in the extension of Definition 3 that we introduced in the previous chapter.

4.1 Dynamics of the $\mathcal{G}_{\mathrm{T}}-$invariant density operator

Having established the formalism of the thermodynamic group in Chapter 3, we now possess the fundamental principles necessary for constructing thermodynamic quantities within this framework. However, there remains a crucial element to characterize: the dynamics of the density matrix invariant under the thermodynamic group.

Since our quantum thermodynamic description is fundamentally emergent, the effective density operator in our formalism must be obtained through coarse-graining of the conventional density operator. Consequently, it is the dynamics of this effective density operator that becomes relevant in our approach.

With this in mind, we shall derive the dynamical equation for this operator, denoted as:

$$\rho_{\mathcal{G}}(t) = \int dg\, V_t \rho(t) V_t^{\dagger} \tag{4.1}$$

where $\rho(t)$ represents the conventional system operator without coarse-graining. In general, the density operator dynamics follows from Eq. (2.24):

$$\frac{d\rho(t)}{dt} = -i\hbar[H(t), \rho] + \mathcal{D}[\rho(t)] \tag{4.2}$$

Taking the Haar average of this expression yields:

$$\begin{aligned} \int dg\, V_t \frac{d\rho(t)}{dt} V_t^{\dagger} &= -i\hbar \int dg\, V_t [H(t), \rho] V_t^{\dagger} + \int dg\, V_t \mathcal{D}[\rho(t)] V_t^{\dagger} \\ &= -i\hbar \left[H(t), \rho_{\mathcal{G}}(t)\right] + \mathcal{D}_{\text{inv}}[\rho(t)] \end{aligned} \tag{4.3}$$

where $\mathcal{D}_{\text{inv}}[\rho(t)] \equiv \int dg\, V_t \mathcal{D}[\rho(t)] V_t^{\dagger}$, since:

$$\int dg\, V_t [H(t), \rho] V_t^{\dagger} = \left[H(t), \int dg\, V_t \rho V_t^{\dagger}\right] = [H(t), \rho_{\mathcal{G}}(t)] \tag{4.4}$$

On the other hand, the time derivative of $\rho_{\mathcal{G}}(t)$ gives:

$$\begin{aligned} \frac{d\rho_{\mathcal{G}}(t)}{dt} &= \frac{d}{dt} \int dg\, V_t \rho(t) V_t^{\dagger} \\ &= \int dg\, V_t \frac{d\rho(t)}{dt} V_t^{\dagger} + \int dg \left(\dot{V}_t \rho(t) V_t^{\dagger} + V_t \rho(t) \dot{V}_t^{\dagger}\right) && (4.5) \\ &= -i\hbar[H(t), \rho_{\mathcal{G}}(t)] + \mathcal{D}_{\text{inv}}[\rho(t)] + \mathcal{L}(\rho) && (4.6) \end{aligned}$$

where the term $\mathcal{L}(\rho)$ is defined as:

$$\mathcal{L}(\rho) \equiv \int dg \left(\dot{V}_t \rho(t) V_t^{\dagger} + V_t \rho(t) \dot{V}_t^{\dagger}\right) \tag{4.7}$$

Thus, the effective operator dynamics governed by Eq. (4.6) applies to open systems under the Markovian approximation. However, our primary interest lies in closed systems, where Eq. (4.6) reduces to:

$$\frac{d\rho_{\mathcal{G}}(t)}{dt} = -i\hbar[H(t), \rho_{\mathcal{G}}(t)] + \mathcal{L}(\rho) \tag{4.8}$$

Remarkably, the dynamics of the thermodynamic group-invariant operator becomes non-unitary, with $\mathcal{L}(\rho)$ acting as an effective dissipator. This implies that the coarse-graining procedure induces non-unitary effects in the density operator dynamics, analogous to those caused by coupling to a reservoir. However, in this case, the $\mathcal{L}(\rho)$ contribution directly reflects modifications in the gauge group structure, manifested through the time derivatives of the transformations V_t

in Eq. (4.8).

In the following sections, we will develop the invariant notions of heat, work, and entropy, subsequently connecting these expressions with the effective density operator dynamics described by Eq. (4.8). This connection will enable us to establish a consistent physical interpretation for these thermodynamic quantities within our framework.

4.2 First law in gauge invariant quantum thermodynamics

The definition of invariant quantities under the thermodynamic group, as well as the Haar average of the elements of the thermodynamic group, is the starting point for obtaining the invariant counterparts associated with any functionals. In this sense, we will now construct the first law of thermodynamics in an invariant form over the thermodynamic group and the Haar average associated with the functionals. For this, we can use Definition 3 applied to the usual notions of work Eq. (2.30) and usual heat Eq. (2.29). Here, the label u introduced in Section 2.2 becomes non-trivial and differentiates the new functionals obtained. These results are initially presented in [3], which are given the following Theorem.

Theorem 1. ***(Gauge-Invariant Work).*** *Let $H(t)$ be a time-dependent Hamiltonian whose decomposition is given by Eq. (3.25), and let u_t be the diagonalizing unitary matrix of the Hamiltonian, i.e., $H(t) = u_t h(t) u_t^\dagger$, where $h(t)$ is differentiable for all $t \in \mathbb{R}$. Then, the notion of work that is invariant with respect to the thermodynamic gauge group is given by*

$$W_{inv}\left[\rho\right] = \int_0^\tau \mathrm{dt}\,\mathrm{Tr}\left\{\rho u_t \dot{h} u_t^\dagger\right\}. \tag{4.9}$$

Proof. Firstly, we derive the notion of invariant work and, subsequently, we obtain the invariant heat. In this sense, from Definition 3 of invariant quantities, the invariant work is given by

$$\begin{aligned} W_{inv}\left[\rho\right] &= \int \mathrm{d}\mathcal{G}_\mathrm{T}\, W_u\left[V_t \rho V_t^\dagger\right] \\ &= \int \mathrm{d}\mathcal{G}_\mathrm{T} \int_0^\tau \mathrm{dt}\,\mathrm{Tr}\left\{V_t \rho V_t^\dagger \dot{H}\right\} \\ &= \int \mathrm{d}\mathcal{G}_\mathrm{T} \int_0^\tau \mathrm{dt}\,\mathrm{Tr}\left\{\rho u_t \mathcal{V}_t^\dagger u_t^\dagger \dot{H} u_t \mathcal{V}_t u_t^\dagger\right\} \\ &= \int_0^\tau \mathrm{dt}\,\mathrm{Tr}\left\{\rho u_t g_t u_t^\dagger\right\}, \end{aligned} \tag{4.10}$$

where $g_t \equiv \int \mathrm{d}\mathcal{G}_\mathrm{T}\, \mathcal{V}_t^\dagger \left(u_t^\dagger \dot{H} u_t\right) \mathcal{V}_t$. In this case, we commute the Haar integral and the integral over t since, given the continuity of the protocol $g(t)$, it follows that $H(t)$ is modified continuously, as is its eigenbasis.

Now, using the decomposition of the Hamiltonian in Eq. (3.25), We can expand the parentheses above to yield:

$$\begin{aligned} u_t^\dagger \dot{H} u_t &= u_t^\dagger \left(\dot{u}_t h u_t^\dagger + u_t \dot{h} u_t^\dagger + u_t h \dot{u}_t^\dagger \right) u_t \\ &= \dot{h} + u_t^\dagger \dot{u}_t h + h \dot{u}_t^\dagger u_t \\ &= \dot{h} + h \dot{u}_t^\dagger u_t - \dot{u}_t^\dagger u_t h \\ &= \dot{h} + \left[h, \dot{u}_t^\dagger u_t \right]. \end{aligned}$$

Then, the g_t can be write as

$$\begin{aligned} g_t &= \int \mathrm{d}\mathcal{G}_\mathrm{T}\, \mathcal{V}_t^\dagger \left(\dot{h} + \left[h, \dot{u}_t^\dagger u_t \right] \right) \mathcal{V}_t \\ &= \int \mathrm{d}\mathcal{G}_\mathrm{T}\, \mathcal{V}_t^\dagger \dot{h} \mathcal{V}_t + \int \mathrm{d}\mathcal{G}_\mathrm{T}\, \mathcal{V}_t^\dagger \left[h, \dot{u}_t^\dagger u_t \right] \mathcal{V}_t \\ &= \dot{h} \int \mathrm{d}\mathcal{G}_\mathrm{T} \left[\bigoplus_{k=1}^{p} \mathbb{1}_{n_t^k} \right] + [h, b(t)] \end{aligned} \tag{4.11}$$

with $b_t = \left[h, \int \mathrm{d}\mathcal{G}_\mathrm{T}\, \mathcal{V}_t^\dagger \dot{u}_t^\dagger u_t \mathcal{V}_t \right]$. Then, substituting Eq. (4.11) into the expression given by Eq. (4.10) we obtain

$$\begin{aligned} W_{inv}[\rho] &= \int_0^\tau \mathrm{dt}\, \mathrm{Tr} \left\{ \rho u_t b_t u_t^\dagger \right\} \\ &= \int_0^\tau \mathrm{dt}\, \mathrm{Tr} \left\{ \rho u_t \left(\dot{h} \int \mathrm{d}\mathcal{G}_\mathrm{T} \left[\bigoplus_{k=1}^{p} \mathbb{1}_{n_t^k} \right] + [h, b_t] \right) u_t^\dagger \right\} \\ &= \int_0^\tau \mathrm{dt}\, \mathrm{Tr} \left\{ \rho u_t \dot{h} u_t^\dagger \int \mathrm{d}\mathcal{G}_\mathrm{T} \left[\bigoplus_{k=1}^{p} \mathbb{1}_{n_t^k} \right] \right\} + \mathrm{Tr} \left\{ \rho u_t [h, b_t] u_t^\dagger \right\}. \end{aligned} \tag{4.12}$$

Now, we evaluate the two Haar integrals in Eq. (4.12). First, we have

$$\int \mathrm{d}\mathcal{G}_\mathrm{T} \bigoplus_{k=1}^{p} \mathbb{1}_{n_t^k} = \int \mathrm{d}\mathcal{G}_\mathrm{T}\, \mathbb{1}_d = \mathbb{1}_d, \tag{4.13}$$

since the Haar measure is normalized.

From the second Haar integral, let us consider a partition of the interval $[0, \tau]$ into intervals $[t_{i_l}, t_{i_s}]$ such that $\bigcup_{i_q \in L} [t_{i_l}, t_{i_s}] = [0, \tau]$, where L is a set of indices and each set $[t_{i_l}, t_{i_s}]$ corresponds to an interval where the configuration of degeneracies n_t^k of the Hamiltonian is fixed. Consequently, the Haar measure $\mathrm{d}\mathcal{G}_\mathrm{T}$ of the thermodynamic group is fixed in each interval. This decomposition allows us to write

$$\int_0^{\tau} \mathrm{dt} \cdot = \sum_{i_q \in L} \int_{t_{i_l}}^{t_{i_s}} \mathrm{dt} \cdot \tag{4.14}$$

Therefore, the commutator of h and b_t are given by

$$\begin{aligned} \int_0^{\tau} \mathrm{dt}\, \mathrm{Tr} \left\{ \rho u_t \left[h, b_t \right] u_t^\dagger \right\} &= \left[h, \int \mathrm{d}\mathcal{G}_{\mathrm{T}}\, \mathcal{V}_t^\dagger \dot{u}_t^\dagger u_t \mathcal{V}_t \right] \\ &= \sum_{i_q \in L} \int_{t_{ip}}^{t_{i_s}} \mathrm{dt}\, \mathrm{Tr} \left\{ \rho \left[h, \bigoplus_{k=1}^{p} b_k(t) \mathbb{1}_{n_t^k} \right] \right\} \\ &= 0 \end{aligned}$$

where

$$\int \mathrm{d}\mathcal{G}_{\mathrm{T}}\, \mathcal{V}_t^\dagger \dot{u}_t^\dagger u_t \mathcal{V}_t = \bigoplus_{k=1}^{p} b_k(t) \mathbb{1}_{n_t^k} \tag{4.15}$$

for some function $b_k(t)$ since the Haar measure over any unitary subgroup is a diagonal matrix, which commutes with h therefore we obtain $[h, b(t)] = 0$ in each interval $[t_{i_p}, t_{i_s}]$ i.e.

$$[h, b(t)] = \left[h, \bigoplus_{k=1}^{p} b_k(t) \mathbb{1}_{\eta_t^k} \right] = \left[\bigoplus_{k=1}^{p} \lambda_k(t) \mathbb{1}_{\eta_t^k}, \bigoplus_{k=1}^{p} b_k(t) \mathbb{1}_{\eta_t^k} \right] = 0. \tag{4.16}$$

Therefore, substituting Eq. (4.13) and Eq. (4.16) in Eq. (4.12) we obtain the invariant work introduced in Eq. (4.9).

Now, we prove the invariance property of this functional, in fact:

$$\begin{aligned} W_{inv}[V_t \rho V_t^\dagger] &= \int_0^{\tau} \mathrm{dt}\, \mathrm{Tr} \left[V_t \rho V_t^\dagger u_t \dot{h} u_t^\dagger \right] \\ &= \int_0^{\tau} \mathrm{dt}\, \mathrm{Tr} \left[\rho u_t \mathcal{V}_t^\dagger \dot{h} \mathcal{V}_t u_t^\dagger \right] \\ &= \int_0^{\tau} \mathrm{dt}\, \mathrm{Tr} \left[\rho u_t \dot{h} u_t^\dagger \right] = W_{inv}[\rho] \end{aligned} \tag{4.17}$$

since $\mathcal{V}_t^\dagger \dot{h} \mathcal{V}_t = \mathcal{V}_t^\dagger \mathcal{V}_t \dot{h} = \dot{h}$. Therefore, the invariant work is invariant under the gauge transformation as desired and this finish this proof. □

In sequence, we formally introduce the expression for the invariant heat in the following theorem.

Theorem 2. *(Gauge-invariant Heat) Over the same assumptions of the invariant work Theorem 1. Then the notion of heat which is invariant with respect to the thermodynamic gauge is given by*

$$Q_{inv}[\rho] = Q_u[\rho] + Q_c[\rho] \tag{4.18}$$

where $Q_u[\rho]$ is the usual heat defined in Eq. (2.29) and

$$Q_c[\rho] \equiv \int_0^{\tau} \mathrm{dt}\, \mathrm{Tr}\left\{\rho \dot{u}_t h u_t^{\dagger} + \rho u_t h \dot{u}_t^{\dagger}\right\} \tag{4.19}$$

is the coherent heat.

Proof. In fact this proof is similar to Theorem 1. Indeed, using the Definition 3 we have

$$\begin{aligned} Q_{inv}\left[\rho\right] &= \int \mathrm{d}\mathcal{G}_{\mathrm{T}}\, Q_u\left[V_t \rho V_t^{\dagger}\right] \\ &= \int \mathrm{d}\mathcal{G}_{\mathrm{T}} \int_0^{\tau} \mathrm{dt}\, \mathrm{Tr}\left\{\frac{\mathrm{d}}{\mathrm{dt}}\left(V_t \rho V_t^{t}\right) H\right\} \\ &= \int \mathrm{d}\mathcal{G}_{\mathrm{T}} \int_0^{\tau} \mathrm{dt}\, \mathrm{Tr}\left\{\left(\dot{V}_t \rho V_t^{\dagger} + V_t \dot{\rho} V_t^{\dagger} + V_t \rho \dot{V}_t^{\dagger}\right) H\right\} \\ &= I_1 + I_2 \end{aligned} \tag{4.20}$$

where I_1 and I_2 are defined by

$$\begin{cases} I_1 \equiv \int \mathrm{d}\mathcal{G}_{\mathrm{T}} \int_0^{\tau} \mathrm{dt}\, \mathrm{Tr}\left\{\left(V_t \dot{\rho} V_t^{\dagger}\right) H\right\} \\ I_2 \equiv I_3 + I_4, \text{ where} \\ I_3 \equiv \int \mathrm{d}\mathcal{G}_{\mathrm{T}} \int_0^{\tau} \mathrm{dt}\, \mathrm{Tr}\left\{\left(\dot{V}_t \rho V_t^{\dagger}\right) H\right\} \\ I_4 \equiv \int \mathrm{d}\mathcal{G}_{\mathrm{T}} \int_0^{\tau} \mathrm{dt}\, \mathrm{Tr}\left\{\left(V_t \rho \dot{V}_t^{\dagger}\right) H\right\} \end{cases} . \tag{4.21}$$

For simplicity, i will subsequently treat each term separately. Firstly, for I_1 we have:

$$\begin{aligned} I_1 &= \int \mathrm{d}\mathcal{G}_{\mathrm{T}} \int_0^{\tau} \mathrm{dt}\, \mathrm{Tr}\left\{V_t \dot{\rho} V_t^{\dagger} H\right\} \\ &= \int \mathrm{d}\mathcal{G}_{\mathrm{T}} \int_0^{\tau} \mathrm{dt}\, \mathrm{Tr}\left\{\dot{\rho} H\right\} \\ &= \int_0^{\tau} \mathrm{dt}\, \mathrm{Tr}\left\{\dot{\rho} H\right\} = Q_u[\rho], \end{aligned} \tag{4.22}$$

since the Haar measure is normalized. Therefore the first term in Eq. (4.20) is the usual heat defined in Eq. (2.29). We must now evaluate I_2 and I_3 for this, we compute the following derivatives of V_t and $V_t^\dagger$:

$$\begin{aligned}
\dot{V}_t &= \frac{\mathrm{d}}{\mathrm{dt}}\left(u_t\mathcal{V}_tu_t^\dagger\right) = \dot{u}_t\mathcal{V}_tu_t^\dagger + u_t\dot{\mathcal{V}}_tu_t^\dagger + u_t\mathcal{V}_t\dot{u}_t^\dagger && (4.23)\\
\dot{V_t^\dagger} &= \frac{\mathrm{d}}{\mathrm{dt}}\left(u_t\mathcal{V}_t^\dagger u_t^\dagger\right) = \dot{u}_t\mathcal{V}_t^\dagger u_t^\dagger + u_t\dot{\mathcal{V}_t^\dagger}u_t^\dagger + u_t\mathcal{V}_t^\dagger\dot{u}_t^\dagger. && (4.24)
\end{aligned}$$

Firstly, for I_3 we have

$$\begin{aligned}
I_3 &= \int \mathrm{d}\mathcal{G}_\mathrm{T}\int_0^T \mathrm{dt}\,\mathrm{Tr}\left\{\left(\dot{V}_t\rho V_t^\dagger\right)H\right\}\\
&= \int \mathrm{d}\mathcal{G}_\mathrm{T}\int_0^\tau \mathrm{dt}\,\mathrm{Tr}\left\{\rho V_tH\left[\dot{u}_t\mathcal{V}_tu_t^\dagger + u_t\dot{\mathcal{V}}_tu_t^\dagger + u_t\mathcal{V}_t\dot{u}_t^\dagger\right]\right\}\\
&= \int \mathrm{d}\mathcal{G}_\mathrm{T}\int_0^\tau \mathrm{dt}\,\mathrm{Tr}\left\{\rho u_t\mathcal{V}_t^\dagger hu_t^\dagger\left[\dot{u}_t\mathcal{V}_tu_t^\dagger + u_t\dot{\mathcal{V}}_tu_t^\dagger + u_t\mathcal{V}_t\dot{u}_t^\dagger\right]\right\}\\
&= \int \mathrm{d}\mathcal{G}_\mathrm{T}\int_0^\tau \mathrm{dt}\,\mathrm{Tr}\left\{\rho\left[u_t\mathcal{V}_t^\dagger h\dot{\mathcal{V}}_tu_t^\dagger + u_t\mathcal{V}_t^\dagger hu_t^\dagger\dot{u}_t\mathcal{V}_tu_t^\dagger\right]\right\} +\\
&+ \int \mathrm{d}\mathcal{G}_\mathrm{T}\int_0^\tau \mathrm{dt}\,\mathrm{Tr}\left\{\rho u_t\mathcal{V}_t^\dagger h\mathcal{V}_t\dot{u}_t^\dagger\right\}. && (4.25)
\end{aligned}$$

The development for I_4 is similar, in effect we have:

$$\begin{aligned}
I_4 &\equiv \int \mathrm{d}\mathcal{G}_\mathrm{T}\int_0^\tau \mathrm{dt}\,\mathrm{Tr}\left\{\left(V_t\rho\dot{V_t^\dagger}\right)H\right\}\\
&= \int \mathrm{d}\mathcal{G}_\mathrm{T}\int_0^\tau \mathrm{dt}\,\mathrm{Tr}\left\{\rho\left[\dot{u}_t\mathcal{V}_t^\dagger u_t^\dagger + u_t\dot{\mathcal{V}_t^\dagger}u_t^\dagger + u_t\mathcal{V}_t^\dagger\dot{u}_t^\dagger\right]u_thu_t^\dagger u_t\mathcal{V}_tu_t^\dagger\right\}\\
&= \int \mathrm{d}\mathcal{G}_\mathrm{T}\int_0^\tau \mathrm{dt}\,\mathrm{Tr}\left\{\rho\left[u_t\dot{\mathcal{V}}_t^\dagger h\mathcal{V}_tu_t^\dagger + u_t\mathcal{V}_t^\dagger\dot{u}_t^\dagger u_th\mathcal{V}_tu_t^\dagger\right]\right\} +\\
&+ \int \mathrm{d}\mathcal{G}_\mathrm{T}\int_0^\tau \mathrm{dt}\,\mathrm{Tr}\left\{\rho\dot{u}_thu_t^\dagger\right\}. && (4.26)
\end{aligned}$$

Then, substituting Eq. (4.25) and Eq. (4.26) in I_2 we obtain:

$$\begin{aligned}
I_2 &= I_3 + I_4\\
&= \int \mathrm{d}\mathcal{G}_\mathrm{T}\int_0^\tau \mathrm{dt}\,\mathrm{Tr}\left\{\rho u_th\dot{u}_t^\dagger\right\} + \int \mathrm{d}\mathcal{G}_\mathrm{T}\int_0^\tau \mathrm{dt}\,\mathrm{Tr}\left\{\rho\dot{u}_thu_t^\dagger\right\} +\\
&+ \int \mathrm{d}\mathcal{G}_\mathrm{T}\int_0^\tau \mathrm{dt}\,\mathrm{Tr}\left\{\rho\left[u_t\mathcal{V}_t^\dagger h\dot{\mathcal{V}}_tu_t^\dagger + u_t\mathcal{V}_t^\dagger hu_t^\dagger\dot{u}_t\mathcal{V}_tu_t^\dagger\right]\right\} +\\
&+ \int \mathrm{d}\mathcal{G}_\mathrm{T}\int_0^\tau \mathrm{dt}\,\mathrm{Tr}\left\{\rho\left[u_t\dot{\mathcal{V}}_t^\dagger h\mathcal{V}_tu_t^\dagger + u_t\mathcal{V}_t^\dagger\dot{u}_t^\dagger u_th\mathcal{V}_tu_t^\dagger\right]\right\}\\
&= \int_0^\tau \mathrm{dt}\,\mathrm{Tr}\left\{\rho\left[u_th\dot{u}_t^\dagger + \dot{u}_thu_t^\dagger\right]\right\}\int \mathrm{d}\mathcal{G}_\mathrm{T}\,\mathbb{1}_{n_t^k} + Q_d[\rho]\\
&= Q_c[\rho] + Q_d[\rho] && (4.27)
\end{aligned}$$

where $Q_c[\rho]$ is the coherent heat defined in Eq (4.19) and $Q_d[\rho]$ is given by

$$\begin{aligned} Q_d[\rho] &= \int \mathrm{d}\mathcal{G}_{\mathrm{T}} \int_0^{\tau} \mathrm{dt}\, \mathrm{Tr}\left\{\rho \left[u_t \mathcal{V}_t^{\dagger} h \dot{\mathcal{V}}_t u_t^{\dagger} + u_t \dot{\mathcal{V}}_t^{\dagger} h \mathcal{V}_t u_t^{\dagger}\right]\right\} \\ &+ \int \mathrm{d}\mathcal{G}_{\mathrm{T}} \int_0^{\tau} \mathrm{dt}\, \mathrm{Tr}\left\{\rho \left[u_t \mathcal{V}_t^{\dagger} h u_t^{\dagger} \dot{u}_t \mathcal{V}_t u_t^{\dagger} + u_t \mathcal{V}_t^{\dagger} \dot{u}_t^{\dagger} u_t h \mathcal{V}_t u_t^{\dagger}\right]\right\}. \end{aligned} \tag{4.28}$$

Indeed, let us show $Q_d[\rho] = 0$. Using the unitary property of $\mathcal{V}_t$ and u_t we can write:

$$\begin{aligned} Q_d[\rho] &= \int \mathrm{d}\mathcal{G}_{\mathrm{T}} \int_0^{\tau} \mathrm{dt}\, \mathrm{Tr}\left\{\rho u_t h \left[\mathcal{V}_t^{\dagger} \dot{\mathcal{V}}_t + \dot{\mathcal{V}}_t^{\dagger} \mathcal{V}_t\right] u_t^{\dagger}\right\} + \\ &+ \int \mathrm{d}\mathcal{G}_{\mathrm{T}} \int_0^{\tau} \mathrm{dt}\, \mathrm{Tr}\left\{\rho u_t \left[h \mathcal{V}_t^{\dagger} u_t^{\dagger} \dot{u}_t \mathcal{V}_t - \mathcal{V}_t^{\dagger} u_t^{\dagger} \dot{u}_t \mathcal{V}_t h\right] u_t^{\dagger}\right\} \\ &= \int \mathrm{d}\mathcal{G}_{\mathrm{T}} \int_0^{\tau} \mathrm{dt}\, \mathrm{Tr}\left\{\rho u_t h \frac{d(\mathcal{V}_t \mathcal{V}_t^{\dagger})}{dt} u_t^{\dagger}\right\} + \qquad (4.29) \\ &+ \sum_{i_q \in L} \int_{t_{i_p}}^{t_{i_s}} \mathrm{dt}\, \mathrm{Tr}\left\{\rho u_t \left[h, \int \mathrm{d}\mathcal{G}_{\mathrm{T}}\, \mathcal{V}_t^{\dagger} u_t^{\dagger} \dot{u}_t \mathcal{V}_t\right] u_t^{\dagger}\right\}. \qquad (4.30) \end{aligned}$$

First, since $\mathcal{V}_t \mathcal{V}_t^{\dagger} = \mathbb{1}_d$ the Integral in Eq. (4.29) is zero. The second integral appearing in Eq. (4.30) vanishes due to the application of the Haar average, in fact, note that

$$\int \mathrm{d}\mathcal{G}_{\mathrm{T}}\, \mathcal{V}_t^{\dagger} u_t^{\dagger} \dot{u}_t \mathcal{V}_t = \bigoplus_{k=1}^{p} r(t) \mathbb{1}_{n_t^k} \tag{4.31}$$

for some function $r(t)$ in each interval $[t_{i_l}, t_{i_s}]$ which is constructed in the same way as we did in the proof of the Theorem 1. Therefore, $Q_d = 0$ and I_2 in Eq. (4.27) reduces to Q_c, from this and from Eq. (4.22) the invariant heat in Eq. (4.20) becomes the sum of the usual Q_u and coherent Q_c heat as desired.

Lastly, we proof the invariance of the invariant heat over the gauge transformation, indeed

$$\begin{aligned} Q_{inv}[V_t \rho V_t^{\dagger}] &= Q_u[V_t \rho V_t^{\dagger}] + Q_c[V_t \rho V_t^{\dagger}] \\ &= Q_u[\rho] + Q_c[\rho] + Q_r[\rho] + Q_c[V_t \rho V_t^{\dagger}] \end{aligned} \tag{4.32}$$

where Q_r is defined by:

$$Q_r[\rho] \equiv \int_0^{\tau} \mathrm{dt}\, \mathrm{Tr}\left\{\rho \left[u_t \mathcal{V}_t^{\dagger} h u_t^{\dagger} \dot{u}_t \mathcal{V}_t u_t^{\dagger} + u_t \mathcal{V}_t^{\dagger} \dot{u}_t^{\dagger} u_t h \mathcal{V}_t u_t^{\dagger}\right]\right\}. \tag{4.33}$$

In this sense, we will then show that $\mathcal{Q} \equiv Q_r[\rho] + Q_c[V_t \rho V_t^\dagger]$ is equal to zero. In this sense we expand $Q_r[\rho]$ as follow

$$
\begin{aligned}
Q_r[\rho] &= \int_0^{\mathcal{T}} \mathrm{dt}\, \mathrm{Tr}\left\{\rho\left[u_t \mathcal{V}_t^\dagger h u_t^\dagger \dot{u}_t \mathcal{V}_t u_t^\dagger + u_t \mathcal{V}_t^\dagger \dot{u}_t^\dagger u_t h \mathcal{V}_t u_t^\dagger\right]\right\} \\
&= \int_0^{\mathcal{T}} \mathrm{dt}\, \mathrm{Tr}\left\{\rho\left[V_t^\dagger H \dot{u}_t u_t^\dagger V_t + V_t^\dagger u_t \dot{u}_t^\dagger H V_t\right]\right\} \\
&= \int_0^{\mathcal{T}} \mathrm{dt}\, \mathrm{Tr}\left\{V_t \rho V_t^\dagger \left[H \dot{u}_t u_t^\dagger + u_t \dot{u}_t^\dagger H\right]\right\},
\end{aligned}
\tag{4.34}
$$

and we rewrite $Q_c[V_t \rho V_t^\dagger]$ as:

$$
\begin{aligned}
Q_c[V_t \rho V_t^\dagger] &= \int_0^{\mathcal{T}} \mathrm{dt}\, \mathrm{Tr}\left\{V_t \rho V_t^\dagger \left[\dot{u}_t h u_t^\dagger + u_t h \dot{u}_t^\dagger\right]\right\} \\
&= \int_0^{\mathcal{T}} \mathrm{dt}\, \mathrm{Tr}\left\{V_t \rho V_t^\dagger \left[\dot{u}_t u_t^\dagger H + H u_t \dot{u}_t^\dagger\right]\right\}.
\end{aligned}
\tag{4.35}
$$

Using Eq. (4.34) and Eq. (4.35) we obtain for $\mathcal{Q}$:

$$
\begin{aligned}
\mathcal{Q} &= \int_0^{\mathcal{T}} \mathrm{dt}\, \mathrm{Tr}\left\{V_t \rho V_t^\dagger \left[H \dot{u}_t u_t^\dagger + u_t \dot{u}_t^\dagger H + \dot{u}_t u_t^\dagger H + H u_t \dot{u}_t^\dagger\right]\right\} \\
&= \int_0^{\mathcal{T}} \mathrm{dt}\, \mathrm{Tr}\left\{V_t \rho V_t^\dagger \left[\frac{\mathrm{d}(u_t u_t^\dagger)}{\mathrm{dt}}, H\right]\right\} = 0
\end{aligned}
$$

since u_t is unitary and we have $u_t \dot{u}_t^\dagger = -\dot{u}_t u_t^\dagger$. Thus the invariant heat in Eq. (4.32) becomes invariant under the thermodynamic group. □

4.2.1 The physical meaning of invariant work and heat

In Theorems 1 and 2, we formally introduced the invariant counterparts associated with work and heat, respectively. With this in mind, we will now discuss the physical implications of these quantities in the context of gauge-invariant quantum thermodynamics.

First, note that under the notion of invariance we established, the heat associated with the system is given by the sum of two contributions, which are Q_u and Q_c, defined by Eq. (2.29) and Eq. (4.19), respectively. Indeed, as we discussed in Chapter 2, the usual heat Q_u, initially introduced in the seminal work of Alicki in Ref.[15], describes the amount of heat exchanged between the environment and the system over a given protocol. Furthermore, as we showed in Chapter 2, closed systems, i.e., under unitary evolution, do not exchange heat with the environment; consequently, we have $Q_u = 0$ in closed systems.

However, note that the invariant heat in Eq. (4.18) is not necessarily zero in the case of a closed system. In fact, in this scenario, the formalism introduced in Chapter 3 for invariant quantities indicates that throughout a given dynamics, whether unitary or not, the energy part of the system referred to as heat has another contribution, which we denote as Q_c.

The term Q_c introduced in Eq. (4.19) was originally derived in the work of Céleri and Rudnicki in Ref.[3] using the gauge invariance of the first law of thermodynamics as per Definition 1. In this work, the authors showed that such a contribution emerges as a consequence of the production of coherence in the energy basis. In fact, expanding Q_c with the density operator in the energy basis $\{|a_n(t)\rangle\}$ given by $\rho(t) = \sum_{j,k} \rho^E_{j,k}(t) |a_j\rangle \langle a_k|$, we obtain:

$$\begin{aligned}
Q_c[\rho(t)] &= \int_0^\tau \mathrm{dt}\, \mathrm{Tr}\left\{\rho(t)\left(\dot{u}_t h u_t^\dagger + u_t h \dot{u}_t^\dagger\right)\right\} \\
&= \int_0^\tau \mathrm{dt}\, \mathrm{Tr}\left\{\sum_{j,k,n} \rho^E_{jk}\lambda_n \left(|\dot{a}_j\rangle\langle a_k| + |a_j\rangle\langle \dot{a}_k|\right)|a_n\rangle\langle a_n|\right\} \\
&= \int_0^\tau \mathrm{dt} \sum_{j,k,n,m} \rho^E_{jk}\left[\lambda_n \langle a_m|\dot{a}_j\rangle \delta_{k,n} + \lambda_n \langle \dot{a}_k|a_n\rangle \delta_{m,j}\right]\delta_{n,m} \\
&= \int_0^\tau \mathrm{dt} \sum_{n,m} \rho^E_{mn}(t) \langle \dot{a}_n(t)|a_m(t)\rangle \left(\lambda_m(t) - \lambda_n(t)\right)
\end{aligned} \tag{4.36}$$

where we changed some dummy labels and used the orthogonality of the state basis $\{|a_n(t)\rangle\}$ such that we have:

$$\langle a_n|a_m\rangle = \delta_{n,m} \implies \frac{\mathrm{d}(\langle a_n|a_m\rangle)}{\mathrm{dt}} = 0 \implies \langle a_n|\dot{a}_m\rangle = -\langle \dot{a}_n|a_m\rangle. \tag{4.37}$$

In summary, note that the expression for Q_c in Eq. (4.36) depends only on the terms associated with the coherences in the energy basis, thus justifying the designation of the quantity Q_c as coherent heat [3]. As a consequence, coherent heat emerges as a result of the transitions that occur in the energy basis, which are fundamentally connected to irreversibility (heat generation) [3].

This discussion reveals the connection between the Q_c term and quantum coherences. However, it is the effective density operator dynamics that demonstrates this energy contribution must be interpreted as heat rather than some peculiar form of "work" or "friction". Indeed, starting from Alicki's thermodynamics, we obtain that the heat associated with the effective state dynamics is given by:

$$\begin{aligned}
Q_u[\rho_{\mathcal{G}}(t)] &= \int_0^\tau dt\, \mathrm{Tr}\left\{H(t)\frac{d\rho_{\mathcal{G}}(t)}{dt}\right\} \\
&= \int_0^\tau dt\, \mathrm{Tr}\left\{H(t)\left[-i\hbar[H(t), \rho_{\mathcal{G}}(t)] + \mathcal{L}(\rho)\right]\right\} \\
&= \int_0^\tau dt\, \mathrm{Tr}\left\{H(t)\mathcal{L}(\rho)\right\} = Q_c[\rho(t)]
\end{aligned} \tag{4.38}$$

where the conclusion in the last line follows from identifying the $\mathcal{L}(\rho)$ term in the integral with the expression obtained for the I_2 term given in Eq. (4.21).

The result in Eq. (4.38) shows that the coherent heat associated with a state $\rho(t)$ is equivalent to the Alicki heat of an effective state $\rho_{\mathcal{G}}(t)$ under the non-unitary effective dynamics given by Eq. (4.8). This allows us to understand the physical meaning of the $Q_c[\rho(t)]$ term, which is fundamentally an effective heat contribution emerging from the coarse-graining over unitary transformations V_t that preserve the Hamiltonian symmetries.

That is, the Haar-average coarse-graining induces effective dissipation that can be attributed to an effective thermal bath. The associated heat is given by the $Q_c[\rho(t)]$ term, justifying its physical interpretation as heat. Thus, coherent heat is interpreted as the amount of energy that becomes inaccessible due to measurement limitations on the system. Consequently, this energy loss carries an inherent irreversibility that remains uncontrolled, even in closed systems.

Now, observe that Eq. (4.36) establishes that coherent heat explicitly depends on both the energy-basis coherences and changes in the energy eigenstates. Given our interpretation of coherent heat, we can attribute this to how system accessibility limitations induce heat generation that manifests through both quantum coherence production in the energy basis and non-adiabatic changes in the energy basis. Note in Eq. (4.36) that only coherences survive the summation (since $\lambda_m - \lambda_n = 0$ when $n = m$), and in the adiabatic regime $|\dot{a}_n(t)\rangle \approx 0$ nullifies this contribution.

Therefore, coherent heat emerges as a direct manifestation of quantum information access limitations, linking irreversibility, coherence production, and non-adiabaticity even in closed systems.

Let us now discuss the physical meaning of the quantity associated with invariant work. In this context, we again turn to Alicki's thermodynamics, where the work associated with the effective state dynamics yields:

$$
\begin{aligned}
W_u[\rho_{\mathcal{G}}(t)] &= \int_0^{\tau} dt\,\mathrm{Tr}\left\{\rho_{\mathcal{G}}(t)\frac{dH}{dt}\right\} \\
&= \int_0^{\tau} dt\,\mathrm{Tr}\left\{\left(\int \mathrm{d}\mathcal{G}_{\mathrm{T}}\, V_t\rho(t)V_t^{\dagger}\right)\frac{dH}{dt}\right\} \\
&= \int \mathrm{d}\mathcal{G}_{\mathrm{T}} \int_0^{\tau} dt\,\mathrm{Tr}\left\{\left(V_t\rho(t)V_t^{\dagger}\right)\frac{dH}{dt}\right\} \\
&= \int \mathrm{d}\mathcal{G}_{\mathrm{T}}\, W_u[V_t\rho(t)V_t^{\dagger}] = W_{inv}[\rho(t)].
\end{aligned}
\tag{4.39}
$$

This result shows that the invariant work for a state $\rho(t)$ corresponds to the standard Alicki work associated with the effective state after coarse-graining. Consequently, there remains no doubt that the contribution we call invariant work should indeed be interpreted as work. Fundamentally, the invariant work represents the effective work emerging from our limited access to the system.

Furthermore, we can establish a connection between invariant work and coherent heat, which provides deeper insight into how the Haar-average coarse-graining redistributes energy contributions within the system. Starting from the invariant work expression:

$$\begin{aligned}
W_{inv}[\rho(t)] &= \int \mathrm{d}\mathcal{G}_{\mathrm{T}} \int_0^\tau dt\, \mathrm{Tr}\left\{\left(V_t\rho(t)V_t^\dagger\right)\frac{dH}{dt}\right\} = \int \mathrm{d}\mathcal{G}_{\mathrm{T}} \int_0^\tau dt\, \mathrm{Tr}\left\{\rho(t)V_t^\dagger\frac{dH}{dt}V_t\right\} \\
&= \int \mathrm{d}\mathcal{G}_{\mathrm{T}} \int_0^\tau dt\, \mathrm{Tr}\left\{\rho(t)\left[\frac{d}{dt}\left(V_t^\dagger H V_t\right) - \dot{V}_t^\dagger H V_t - V_t^\dagger H \dot{V}_t\right]\right\} \\
&= \int \mathrm{d}\mathcal{G}_{\mathrm{T}} \int_0^\tau dt\, \mathrm{Tr}\left\{\rho(t)\frac{dH}{dt}\right\} - \int \mathrm{d}\mathcal{G}_{\mathrm{T}} \int_0^\tau dt\, \mathrm{Tr}\left\{\rho(t)\left[\dot{V}_t^\dagger H V_t + V_t^\dagger H \dot{V}_t\right]\right\} \\
&= \int \mathrm{d}\mathcal{G}_{\mathrm{T}} \int_0^\tau dt\, \mathrm{Tr}\left\{\rho(t)\frac{dH}{dt}\right\} - \int_0^\tau dt\, \mathrm{Tr}\left\{H\left[\int \mathrm{d}\mathcal{G}_{\mathrm{T}}\, V_t\rho(t)\dot{V}_t^\dagger + \dot{V}_t\rho(t)V_t^\dagger\right]\right\} \\
&= \int_0^\tau dt\, \mathrm{Tr}\left\{\rho(t)\frac{dH}{dt}\right\} - \int_0^\tau dt\, \mathrm{Tr}\left\{H\mathcal{L}(\rho)\right\} \\
&= W_u[\rho(t)] - Q_c[\rho(t)].
\end{aligned}$$

We thus obtain the fundamental relation:

$$W_{inv}[\rho(t)] = W_u[\rho(t)] - Q_c[\rho(t)], \tag{4.40}$$

The equality in Eq. (4.40) reveals crucial aspects of our approach, particularly concerning the physical interpretation of both invariant work and coherent heat. To properly evaluate Eq. (4.40), we must first understand the role of the coherent heat sign. Three distinct possibilities emerge:

- $Q_c[\rho(t)] > 0$. In this case, $Q_c[\rho(t)]$ is strictly positive, and consequently:

  $$W_{inv}[\rho(t)] < W_u[\rho(t)].$$

  This represents the physical situation where information limitations about the system manifest as effective dissipation. Here, part of the energy previously interpreted as work becomes inaccessible, necessitating that the effective work be strictly less than the conventional work predicted by Alicki's framework. This case further emphasizes how $Q_c[\rho(t)]$ embodies irreversibility in closed systems, where this contribution reduces the extractable work from the system. An immediate consequence is the diminished efficiency of quantum thermal machines operating under such conditions.

- $Q_c[\rho(t)] = 0$. This scenario arises under specific conditions. First, when the Hamiltonian is time-independent or more precisely, when its eigenstates are time-independent. Here, the matrices u_t become effectively constant, eliminating non-adiabatic effects and consequently nullifying coherent heat, making the invariant work equivalent to conventional work:

$$W_{inv}[\rho(t)] = W_u[\rho(t)].$$

Another possibility is adiabatic evolution, where by similar reasoning the coherent heat vanishes. A particularly important case occurs in the thermodynamic limit. From Eq. (4.40), we explicitly derive the coherent heat expression:

$$\begin{aligned} Q_c[\rho(t)] &= W_u[\rho(t)] - W_{inv}[\rho(t)] \\ &= \int_0^\tau dt\,\mathrm{Tr}\left\{\rho(t)\frac{dH}{dt}\right\} - \int_0^\tau dt\,\mathrm{Tr}\left\{\rho(t)u_t\frac{dh}{dt}u_t^\dagger\right\} \\ &= \int_0^\tau dt\,\mathrm{Tr}\left\{\rho(t)\left[\frac{dH}{dt} - u_t\frac{dh}{dt}u_t^\dagger\right]\right\} \end{aligned} \tag{4.41}$$

which describes coherent heat as the difference between the total Hamiltonian's time derivative and that of the energy-basis diagonal Hamiltonian. In the thermodynamic limit, these quantities coincide as basis-dependent notions vanish, yielding $Q_c[\rho(t)] \to 0$.

- $Q_c[\rho(t)] < 0$. This subtle case requires careful analysis. Here, the work relation becomes:

  $$W_{inv}[\rho(t)] > W_u[\rho(t)]$$

  representing enhanced work extraction despite informational constraints. We expect this situation only under specific circumstances. First, in finite-dimensional Hilbert spaces where state dynamics may permit periodic returns to initial conditions, potentially releasing quantum coherences that render coherent heat negative. Additionally, optimal control protocols may provide alternative pathways to achieve $Q_c[\rho(t)] < 0$.

Through this analysis, we establish the physical meaning of invariant heat and work while demonstrating how energy relations consistently satisfy the first law framework. Indeed, Eqs. (4.38), (4.39), and (4.40) yield the following equivalent formulations of the first law within the $\mathcal{G}_{\mathrm{T}}$ group thermodynamics:

$$\Delta\,\mathrm{U}[\rho(t)] = W_u[\rho(t)] + Q_u[\rho(t)] \tag{4.42}$$

$$= W_u[\rho_{\mathcal{G}}(t)] + Q_u[\rho_{\mathcal{G}}(t)] \tag{4.43}$$

$$= W_{inv}[\rho(t)] + Q_u[\rho(t)] + Q_c[\rho(t)] \tag{4.44}$$

ensuring thermodynamic consistency in our formalism. This emerges naturally from the gauge invariance principle formulated through mean energy invariance according to Definition 3. The proofs of Theorems 1 and 2 explicitly show that invariant quantities require Haar averaging over the thermodynamic group at each time interval. Furthermore, the differentiability of energy eigenbasis vectors proves essential for deriving the invariant heat and work expressions.

This discussion gains particular relevance by clarifying how the gauge theory formalism of the thermodynamic group $\mathcal{G}_T$, developed by Céleri and Rudnicki in Ref. [3], fundamentally enables these results.

Another noteworthy aspect concerns the absence of quantum coherences in invariant quantities. Indeed, Eq. (4.40) reveals that invariant work corresponds to the conventional work contribution devoid of energy-basis coherences. This becomes explicit when expanding the invariant work term:

$$\begin{aligned}
W_{inv}[\rho] &= \int_0^\tau dt\,\mathrm{Tr}\left\{\rho^E \dot{h}\right\} \\
&= \int_0^\tau dt\,\mathrm{Tr}\left\{\sum_{j,k,n} \rho^E_{jk}\dot{\lambda}_n \left|a_j\right\rangle\left\langle a_k\right| \left(\left|a_n\right\rangle\left\langle a_n\right| + \frac{d}{dt}(\left|a_n\right\rangle\left\langle a_n\right|)\right)\right\} \\
&= \int_0^\tau dt \sum_{j,n,m} \rho^E_{jn}\dot{\lambda}_n \rho^E_{jk}\delta_{j,m}\delta_{k,m} \\
&= \int_0^\tau dt \sum_n \rho^E_{nn}(t)\dot{\lambda}_n(t).
\end{aligned} \tag{4.45}$$

This result underscores how the coarse-graining procedure systematically treats energy contributions from quantum coherences as a distinct energy form—specifically, as heat.

Remarkably, while coherent heat relates to energy-basis coherence production, both invariant heat and work remain coherence-independent. For invariant heat:

$$\begin{aligned}
Q_{inv}\left[\rho\right] &= \int_0^\tau dt\,\mathrm{Tr}\left\{H\dot{\rho}\right\} + \mathrm{Tr}\left\{\rho\dot{u}_t h u_t^\dagger + \rho u_t h \dot{u}_t^\dagger\right\} \\
&= \int_0^\tau dt\,\mathrm{Tr}\left\{h\frac{d}{dt}\left(u_t^\dagger \rho u_t\right)\right\} \\
&= \int_0^\tau dt\,\mathrm{Tr}\left\{\sum_{j,k,n} \lambda_n(t)\left|a_k\right\rangle\left\langle a_k\right| \left(\dot{\rho}^E_{jk}\left|a_j\right\rangle\left\langle a_k\right| + \frac{d(\left|a_j\right\rangle\left\langle a_k\right|)}{dt}\right)\right\} \\
&= \int_0^\tau dt \sum_n \lambda_n(t)\dot{\rho}^E_{nn}(t).
\end{aligned} \tag{4.46}$$

The energy expectation value similarly exhibits coherence independence:

$$\mathrm{U} = \mathrm{Tr}\{\rho H\} = \mathrm{Tr}\{\rho^E h\} = \sum_n \rho^E_{nn}(t)\lambda_n(t). \tag{4.47}$$

The results in Eqs. (4.45)-(4.47) align with classical thermodynamic expectations [3], where work and heat fundamentally derive from population dynamics rather than coherence. This coherence independence in our invariant quantities contrasts with standard quantum thermodynamics frameworks [3], yet precisely mirrors classical energy-exchange notions that inherently disregard quantum coherences.

4.2.2 Covariant derivative and their properties

In the sense of the Gauge theory like introduced in the Section 3.1 we going to introduce another interesting element here, indeed, the notion of covariant derivative and we analyze some properties of this covariant derivative. Then, the formal notion of covariant derivative are introduced in the following definition.

Definition 6. *(Covariant derivative) Let us introduce a Hermitian potential* $A_t \equiv i\dot{u}_t u_t^\dagger$*. Then, we can deine the covariant derivative by:*

$$\begin{aligned} \nabla_{\mathrm{t}} : \mathcal{L}(\mathcal{H}^d) \;&\rightarrow\; \mathcal{L}(\mathcal{H}^d) \\ \phi \in \mathcal{L}(\mathcal{H}^d) \;&\rightarrow\; \nabla_{\mathrm{t}}(\phi) = \frac{\partial}{\partial t}(\phi) + i[A_t, \phi] \end{aligned} \tag{4.48}$$

for all operator $\phi \equiv \phi(t)$*, where* $\mathcal{L}(\mathcal{H})$ *is the vector space of the bounded operators in* $\mathcal{H}^d$*.*

Proposition 5. *(Transformation of covariant derivative). The covariant derivative operator, defined in Eq. (4.48), transforms under the emergent gauge transformation* V_t *as follows:*

$$\nabla_{\mathrm{t}}(\phi) \;\rightarrow\; \nabla_{\mathrm{t}}{}'(\phi) = V_t^\dagger \left[\nabla_{\mathrm{t}}(V_t \phi V_t^\dagger)\right] V_t = \frac{\partial \phi}{\partial t} + i[A'_t, \phi] \tag{4.49}$$

where $A'_t \equiv V_t^\dagger A_t V_t - iV_t^\dagger \dot{V}_t$*.*

Proof.

$$\begin{aligned} \nabla_{\mathrm{t}}\left(V_t \phi V_t^\dagger\right) &= \frac{\partial}{\partial t}\left(V_t \phi V_t^\dagger\right) + i\left[A_t, V_t \phi V_t^\dagger\right] \\ &= \dot{V}_t \phi V_t^\dagger + V_t \dot{\phi} V_t^\dagger + V_t \phi \dot{V}_t^\dagger + \left[A_t, V_t \phi V_t^\dagger\right] \\ &= V_t \dot{\phi} V_t^\dagger + iV_t\left(V_t^\dagger A_t V_t - iV_t^\dagger \dot{V}_t\right)\phi V_t^\dagger \\ &- iV_t \phi\left(V_t^\dagger A_t V_t - iV_t^\dagger \dot{V}_t\right)V_t^\dagger \\ &= V_t \dot{\phi} V_t^\dagger + iV_t\left(A'_t \phi - \phi A'_t\right)V_t^\dagger \\ &= V_t\left(\dot{\phi} + i\left[A'_t, \phi\right]\right)V_t^\dagger \\ &= V_t\left[\nabla_{\mathrm{t}}{}'(\phi)\right]V_t^\dagger. \end{aligned}$$

Therefore, we have:

$$\nabla_{\mathrm{t}}\left(V_t\phi V_t^{\dagger}\right) = V_t\,\nabla_{\mathrm{t}}{}'\left(\phi\right)V_t^{\dagger} \implies \nabla_{\mathrm{t}}{}'\left(\phi\right) = V_t^{\dagger}\left[\nabla_{\mathrm{t}}\left(V_t\phi V_t^{\dagger}\right)\right]V_t$$

and the result is obtained. □

Theorem 3. *The invariant work and heat can be written as:*

$$W_{inv}[\rho] = \int_0^{\tau} \mathrm{dt}\,\mathrm{Tr}\left\{\rho\,\nabla_{\mathrm{t}}(H)\right\}, \tag{4.50}$$

$$Q_{inv}[\rho] = \int_0^{\tau} \mathrm{dt}\,\mathrm{Tr}\left\{H\,\nabla_{\mathrm{t}}(\rho)\right\}. \tag{4.51}$$

Proof. First, we will derive the expression for the invariant work. Note that obtaining Eq. (4.51) is equivalent to showing that $\nabla_{\mathrm{t}}(H) = u_t\dot{h}u_t^{\dagger}$. Starting from this, we have the following development.

$$\begin{array}{rcl}
\nabla_{\mathrm{t}}(H) & = & \dfrac{\partial}{\partial t}H + i\left[A_t, H\right] \\
 & = & \dfrac{\partial}{\partial t}\left(u_t h u_t^{\dagger}\right) + i\left[A_t, u_t h u_t^{\dagger}\right] \\
 & = & \dot{u}_t h u_t^{\dagger} + u_t\dot{h}u_t^{\dagger} + u_t h\dot{u}_t^{\dagger} + i(A_t u_t h u_t^{\dagger} - u_t h u_t^{\dagger}A_t\Big) \\
 & = & \dot{u}_t h u_t^{\dagger} + u_t\dot{h}u_t^{\dagger} + u_t h\dot{u}_t^{\dagger} - \left(\dot{u}_t h u_t^{\dagger} - u_t h u_t^{\dagger}\dot{u}_t u_t^{\dagger}\right) \\
 & = & u_t\dot{h}u_t^{\dagger} + u_t h\dot{u}_t^{\dagger} + u_t h u_t^{\dagger}\dot{u}_t u_t^{\dagger} \\
 & = & u_t\dot{h}u_t^{\dagger} + u_t h\dot{u}_t^{\dagger} - u_t h\dot{u}_t^{\dagger}u_t u_t^{\dagger} \\
 & = & u_t\dot{h}u_t^{\dagger} + u_t h\dot{u}_t^{\dagger} - u_t h\dot{u}_t^{\dagger} = u_t\dot{h}u_t^{\dagger}
\end{array}$$

therefore $\nabla_{\mathrm{t}}(H) = u_t\dot{h}u_t^{\dagger}$ as wished.

To obtain the expression in Eq. (4.51), we will perform a direct derivation starting from Eq. (4.51). In effect, we have:

$$\begin{aligned}
\int_0^\tau \mathrm{dt}\,\mathrm{Tr}\left\{H\,\nabla_{\mathrm{t}}(\rho)\right\} &= \int_0^\tau \mathrm{dt}\,\mathrm{Tr}\left\{H\dot{\rho}+i\left[A_t,\rho\right]\right\}\\
&= \int_0^\tau \mathrm{dt}\,\mathrm{Tr}\left\{H\dot{\rho}+H\rho\dot{u}_t u_t^\dagger - H\dot{u}_t u_t^\dagger\rho\right\}\\
&= \int_0^\tau \mathrm{dt}\,\mathrm{Tr}\left\{H\dot{\rho}+u_t h u_t^\dagger\rho\dot{u}_t u_t^\dagger - u_t h u_t^\dagger \dot{u}_t^\dagger u^\dagger\rho\right\}\\
&= \int_0^\tau \mathrm{dt}\,\mathrm{Tr}\left\{H\dot{\rho}+\rho\dot{u}_t h u_t^\dagger - \rho u_t h\left(u_t^\dagger\dot{u}_t\right)u_t^\dagger\right\}\\
&= \int_0^\tau \mathrm{dt}\,\mathrm{Tr}\left\{H\dot{\rho}+\rho\dot{u}_t h u_t^\dagger + \rho u_t h\left(\dot{u}_t^\dagger u_t\right)u_t^\dagger\right\}\\
&= \int_0^\tau \mathrm{dt}\,\mathrm{Tr}\left\{H\dot{\rho}+\rho\left(\dot{u}_t h u_t^\dagger + u_t h\dot{u}_t^\dagger\right)\right\}\\
&= Q_u\left[\rho\right]+Q_c\left[\rho\right]\\
&= Q_{inv}[\rho]
\end{aligned}$$

therefore $Q_{inv}[\rho]=\int_0^\tau \mathrm{dt}\,\mathrm{Tr}\left\{H\,\nabla_{\mathrm{t}}(\rho)\right\}$ as desired. □

Corollary 1. *(Invariance of covariant derivative) The invariant work and heat are invariant under the covariant derivative, i.e.*

$$W_{inv}[\rho]=\int_0^\tau \mathrm{dt}\,\mathrm{Tr}\left[\rho\,\nabla_{\mathrm{t}}(H)\right]=\int_0^\tau \mathrm{dt}\,\mathrm{Tr}\left[\rho\,\nabla_{\mathrm{t}}'(H)\right] \tag{4.52}$$

$$Q_{inv}[\rho]=\int_0^\tau \mathrm{dt}\,\mathrm{Tr}\left[H\,\nabla_{\mathrm{t}}(\rho)\right]=\int_0^\tau \mathrm{dt}\,\mathrm{Tr}\left[H\,\nabla_{\mathrm{t}}'(\rho)\right] \tag{4.53}$$

where $\nabla_{\mathrm{t}}'(\cdot)$ are defined in Eq. (4.49).

Proof. It follows from Theorem 1 that W_{inv} is invariant under the thermodynamic group, i.e. $W_{inv}[V_t\rho V_t^\dagger]=W_{inv}[\rho]$. Therefore, we obtain

$$W_{inv}[\rho]=\int_0^\tau \mathrm{dt}\,\mathrm{Tr}\left\{\rho\,\nabla_{\mathrm{t}}\left(H\right)\right\}=W_{\mathrm{inv}}\left[V_t\rho V_t^\dagger\right]=\int_0^\tau \mathrm{dt}\,\mathrm{Tr}\left\{\rho\,\nabla_{\mathrm{t}}'\left(H\right)\right\},$$

with proves Eq. (4.52). On the other hand, note that the invariant heat, expressed in terms of the covariant derivative in Eq. (4.51), under the action of the thermodynamic group, is given by:

$$\begin{aligned}
Q_{inv}[V_t\rho V_t^{\dagger}] &= \int_0^{\tau} \mathrm{dt}\,\mathrm{Tr}\left\{H\,\nabla_{\mathrm{t}}\left(V_t\rho V_t^{\dagger}\right)\right\} \\
&= \int_0^{\tau} \mathrm{dt}\,\mathrm{Tr}\left\{V_t^{\dagger}HV_t\,\nabla_{\mathrm{t}}\left(V_t^{\dagger}\rho V_t\right)\right\} \\
&= \int_0^{\tau} \mathrm{dt}\,\mathrm{Tr}\left\{H\left[V_t^{\dagger}\,\nabla_{\mathrm{t}}\left(V_t\rho V_t^{\dagger}\right)V_t\right]\right\} \\
&= \int_0^{\tau} \mathrm{dt}\,\mathrm{Tr}\left\{H\,\nabla_{\mathrm{t}}{}'\left(\rho\right)\right\}.
\end{aligned}$$

Therefore, using the invariance of heat under the thermodynamic group, i.e $Q_{inv}[V_t\rho V_t^{\dagger}] = Q_{inv}[\rho]$, we obtain

$$Q_{inv}[\rho] = \int_0^{\tau} \mathrm{dt}\,\mathrm{Tr}\left\{H\,\nabla_{\mathrm{t}}(\rho)\right\} = Q_{inv}[V_t\rho V_t^{\dagger}] = \int_0^{\tau} \mathrm{dt}\,\mathrm{Tr}\left\{H\,\nabla_{\mathrm{t}}{}'\left(\rho\right)\right\}$$

and the equality Eq. (4.53) is atingible. □

4.3 Entropy in gauge invariant quantum thermodynamics

Having obtained the new formulations for quantities such as heat and work, we will proceed with the construction of gauge invariant quantum thermodynamics by developing the notion of entropy associated with the second law.

As we discussed in Section 2.3, quantum thermodynamics and, more specifically, information theory have introduced various notions of entropy, which have distinct interpretations and their applicability may be restricted to particular contexts [89]. Consequently, defining the notion of entropy within this formalism involves the choice of a functional related to some entropy that we refer to as the usual one. In particular, we understand that a natural choice is to adopt Von Neumann entropy as the usual entropy.

Indeed, in Chapter 2, we introduced and discussed some concepts of candidates for microscopic thermodynamic entropy. However, note that among the mentioned entropies, Boltzmann entropy is necessarily excluded since we cannot associate it as a functional of the density operator and therefore it does not meet the basic hypotheses of the theory discussed in Chapter 3. On the other hand, note that we can view both observational entropy and diagonal entropy as the application of a modified density operator on Von Neumann entropy.

Thus, the natural choice to be made is Von Neumann entropy, which we interpret as a measure of information in Quantum Mechanics.

Therefore, since the Von Neumann entropy is invariant under unitary transformation we can use the Definition Eq. (3.34) of the invariant quantities to construct the invariant entropy version. In this sense, we formally established this in the following theorem.

Theorem 4. *($\mathcal{G}_{\mathrm{T}}$-entropy) The notion of invariant entropy under the emergent gauge group is the gauge entropy which is denoted as $S_{\mathcal{G}_{\mathrm{T}}}$ and gives by:*

$$S_{\mathcal{G}_{\mathrm{T}}}[\rho(t)] = S_u[\rho^E_{dd}(t)], \tag{4.54}$$

where ρ^E_{dd} is defined in Eq. (3.42).

Proof. First, since the Von Neumann entropy is invariant under the unitary transformation the notion of invariant Von Neumann entropy is given by:

$$S_{\mathcal{G}_{\mathrm{T}}}[\rho(t)] \equiv S_{inv}[\rho(t)] = S_u[\mathrm{D}_{\mathcal{G}_{\mathrm{T}}}](\rho(t))] = S_u[\rho^E_{dd}],$$

with ρ^E_{dd} defined in Eq. (3.42). □

Thus, we finally have the notion of gauge entropy formulated. In this sense, it is now appropriate to explore some properties associated with this entropy. In summary, the main characteristics of gauge entropy are associated with the aspects of the state $\rho^E_{dd}(t)$. In particular, the notion of invariant states that we introduced in Chapter 3 will be of certain relevance in this section.

In fact, gauge entropy is obtained from the Haar integral with the induced measure from the gauge group defined by Eq. (3.31). Consequently, since the Haar integration process is analogous to a type of coarse-graining, we can then define a specific type of coarse-graining given by:

$$\mathcal{C} = \{\Pi_{n^k_t}\}, \tag{4.55}$$

in which each projector $\Pi_{n^k_t}$ is associated with the Hilbert subspace $\mathcal{H}_k$ of the energy basis. Certainly, it is easy to verify that these projectors satisfy the relations:

$$\begin{cases} \Pi_{n^k_t}\Pi_{n^m_t} = \delta_{k,m}\Pi_{n^k_t} \\ \sum\limits_k \Pi_{n^k_t} = \mathbb{1}_d \end{cases} \tag{4.56}$$

where $\delta_{k,m}$ is the Kronecker delta. Thus, the set $\mathcal{C}$ is indeed a coarse-graining as defined in [90, 91]. In this sense, we are motivated to define the volume of each subspace by $V_k = \mathrm{Tr}\{\Pi_{n^k_t}\}$.

With this, the $\mathcal{G}_T$-entropy reduces to the following:

$$\begin{aligned}
S_{\mathcal{G}_\mathrm{T}}[\rho(t)] &= S_u[\rho^E_{dd}(t)] \\
&= -\operatorname{Tr}\left\{\rho^E_{dd}(t)\log(\rho^E_{dd}(t))\right\} \\
&= -\operatorname{Tr}\left\{\frac{\operatorname{Tr}\{\rho^E_{n^k_t}(t)\}}{n^k_t}\Pi_{n^k_t}\log\left[\frac{\operatorname{Tr}\{\rho^E_{n^k_t}(t)\}}{n^k_t}\Pi_{n^k_t}\right]\right\} \\
&= -\sum_{k=1}^{p}\operatorname{Tr}\{\rho^E_{n^k_t}(t)\}\log\left[\frac{\operatorname{Tr}\{\rho^E_{n^k_t}(t)\}}{n^k_t}\right]
\end{aligned}$$

note that $n^k_t = V_k = \operatorname{Tr}\{\Pi_{n^k_t}\}$, then we can writhe the $\mathcal{G}_\mathrm{T}$-entropy as:

$$S_{\mathcal{G}_\mathrm{T}}[\rho(t)] = -\sum_{k=1}^{p}\operatorname{Tr}\{\rho^\mathrm{E}_{\mathrm{n}^\mathrm{k}_\mathrm{t}}(\mathrm{t})\}\log\left[\frac{\operatorname{Tr}\{\rho^E_{n^k_t}(t)\}}{V_k}\right] \tag{4.57}$$

Thus, the $\mathcal{G}_T$-entropy can be expressed similarly to an observational entropy [54] where the "coarse-graining" is defined by Eq. (4.55). Consequently, the derivation of Eq. (4.57) guarantees that the $\mathcal{G}_T$-entropy possesses all the properties that we stated in Section 2.3.3.

However, note that the notion of coarse-graining introduced by the set $\mathcal{C}$ defined in Eq. (4.55) is not necessarily connected to the physical notion of coarse-graining as discussed in Chapter 3. In summary, there is no imposition regarding the possibility that the energy levels are distinguishable. In other words, from a conceptual perspective, even though we can associate the $\mathcal{G}_T$-entropy with observational entropy, we cannot claim that both are equivalent.

Furthermore, the distinction between these two notions of entropy becomes even clearer as we evaluate the $\mathcal{G}_T$-entropy considering invariant states. Indeed, we introduced in Definition 4 the notion of invariant states; consequently, the $\mathcal{G}_T$-entropy for any invariant state ρ_{inv} is such that:

$$S_{\mathcal{G}_\mathrm{T}}[\rho_{inv}] = S_u[D(\rho_{inv})] = S_u[\rho_{inv}(t)]. \tag{4.58}$$

That is, no coarse-graining measurement is applied to the state, and the $\mathcal{G}_T$-entropy reduces to Von Neumann entropy. A particular importance of this discussion arises when we consider the case of states that are invariant under the second condition we presented in Proposition 4, that is, when the states are determined solely by the Hamiltonian operator. Therefore, states described by statistical ensembles, such as the canonical or microcanonical ensemble, are invariant, and thus the description of the $\mathcal{G}_T$-entropy reduces to the Gibbs entropy associated with these distributions.

Therefore, the $\mathcal{G}_T$-entropy is consistent with Gibbs entropy for thermal states in equilibrium. In summary, note that this result is independent of the gauge group, as long as the Haar measure is associated with the Hamiltonian of the system. Thus, we see a subtle difference here between observational entropy, which is consistent with Gibbs entropy for states in thermal equilibrium if and only if there is an appropriate choice of coarse-graining.

Now, we will discuss the continuity of the $\mathcal{G}_T$-entropy. In fact, we know that Von Neumann entropy is a continuous function [41, 50], so it would be natural to expect such behavior for the $\mathcal{G}_T$-entropy. However, note that the state ρ_{dd}^{E} is obtained through a map associated with the quantum twirling operator in Eq. (3.36). Furthermore, the Haar measure induced by the thermodynamic group is associated with a parameter, which can be, for example, time. As a result, certain modifications in the gauge group, equivalently in the distribution of the Hamiltonian's degeneracies, may cause the gauge entropy to exhibit some type of discontinuity.

Still, in this context, we will evaluate some interesting cases. First, note that if we have a time-dependent Hamiltonian $H(t)$ associated with a controllable parameter $g(t)$ that behaves well, then the thermodynamic group will change smoothly, and any possible change in the configuration of degeneracies should not produce any discontinuity in the $\mathcal{G}_T$-entropy. Similarly, if $g(t)$ does not modify the degeneracies of the Hamiltonian, the gauge group remains the same, and thus the gauge entropy should not exhibit any discontinuity.

On the other hand, cases where the parameter $g(t)$ is not well behaved may cause certain discontinuities. In Chapter 5, we present, in one of our applications, a particular case that reveals this behavior. Next, we will discuss how the $\mathcal{G}_T$-entropy relates to diagonal entropy.

4.3.1 $\mathcal{G}_{\mathrm{T}}$-entropy and diagonal entropy

Initially, we showed that the $\mathcal{G}_T$-entropy can be written as an observational-type entropy. However, we can approximate gauge entropy as diagonal entropy, which we understand to be the natural way to comprehend the physical meaning of the $\mathcal{G}_T$-entropy. In this sense, let us begin our discussion by establishing a limiting case for the $\mathcal{G}_T$-entropy that emerges in the absence of degeneracies in the spectrum of the Hamiltonian, which is presented as a corollary of Theorem 4.

Corollary 2. *The $\mathcal{G}_{\mathrm{T}}$-entropy coincides with the diagonal entropy if:*

(a) If a Hamiltonian exhibits no degeneracies,

(b) If a $\rho(t)$ is invariant accordingly to the Definition 4.

Proof. We begin by proving case (a). Indeed, if the Hamiltonian has no degeneracies, the gauge group $\mathcal{G}_{\mathrm{T}}$ can be written as:

$$\mathcal{G}_{\mathrm{T}} = \mathcal{U}(1) \times \ldots \times \mathcal{U}(1) = \prod_{i=1}^{d} \mathcal{U}(1).$$

Therefore, the general expression of the density operator Eq. (3.42) reduces to:

$$\rho^E_{dd}(t) = \bigoplus_{k=1}^{d} \frac{\mathrm{Tr}\left\{\rho^E(t)\,|k\rangle\,\langle k|\right\}}{n^k_t}\mathbb{1}_1 = \rho^E_{diag}(t) \tag{4.59}$$

where ρ^E_{diag} is the density operator with the off-diagonal (in the the energy eigenbasis) elements removed. Therefore, the $\mathcal{G}_{\mathrm{T}}$-entropy becomes:

$$S_{\mathcal{G}_{\mathrm{T}}}[\rho(t)] = S_u[\rho^E_{diag}(t)] = S_d[\rho(t)] \tag{4.60}$$

where $S_d[\rho(t)]$ is the diagonal entropy.

For the case (b), if ρ is a invariant state we have:

$$D[\rho(t)] = \rho \implies \Lambda_{\mathcal{G}_{\mathrm{T}}}[\rho^E(t)] = \rho^E_{diag}(t) \tag{4.61}$$

therefore, the $\mathcal{G}_{\mathrm{T}}$-entropy becomes:

$$S_{\mathcal{G}_{\mathrm{T}}}[\rho(t)] = S_u[\Lambda_{\mathcal{G}_{\mathrm{T}}}[\rho^E(t)]] = S_u[\rho^E_{diag}] = S_d[\rho(t)] \tag{4.62}$$

then, the corollary is proved. □

In general, we are not interested in working with invariant states, as the description becomes redundant. Therefore, in these cases, the diagonal entropy emerges from the $\mathcal{G}_T$-entropy due to the absence of degeneracies, which is consistent with the definition of diagonal entropy since it is well-defined, generally, when the system has no degeneracies or when these are not relevant [28].

Next, we will explore in more detail the relationship between gauge entropy and diagonal entropy. In fact, as we refine this relationship, we will be able to assign a physical meaning to the $\mathcal{G}_T$-entropy, thus allowing us to establish the formulation for the second law in our theory. Therefore, let us consider the following properties of gauge entropy associated with diagonal entropy.

Properties 1. *The following properties holds:*

(iii) The $\mathcal{G}_{\mathrm{T}}$-entropy is greater than the diagonal entropy, i.e.

$$S_{\mathcal{G}_{\mathrm{T}}}[\rho(t)] \geq S_d[\rho(t)]. \tag{4.63}$$

(iv) If there exists at least one non-degenerate level in the spectrum of the Hamiltonian, then the $\mathcal{G}_{\mathrm{T}}$-entropy can be written as:

$$S_{\mathcal{G}_{\mathrm{T}}}[\rho(t)] = S_d[\rho(t)] + S_\Gamma[f_t] \tag{4.64}$$

where $s[f_t] \equiv -\operatorname{Tr}\{f_t \log(|f_t|)\}$ *and* f_t *is a block diagonal matrix given by*

$$f_t = \begin{pmatrix} \begin{pmatrix} \textit{Non degenerate} \\ -\rho^E_{kk}(t) \end{pmatrix} & 0 \\ 0 & \begin{pmatrix} \textit{Degenerate} \\ \dfrac{\operatorname{Tr}\{\rho^E(t)\Pi_{n^k_t}\}}{n^k_t} \end{pmatrix} \end{pmatrix} \tag{4.65}$$

which each block of f_t *is diagonal.*

(v) $S_\Gamma[f_t]$ *defined above is non-negative, i.e* $S_\Gamma[f_t] \geq 0$. *And the equality is saturable if* $\rho(t)$ *is a invariant state accordingly to the Definition 4 or the Hamiltonian spectrum is non degenerated.*

Proof. First, let us demonstrate property (iii). Since the Haar average of an operator is equal to the Haar average of the diagonal part of that same operator (proved in Appendix B.3), it follows that the gauge entropy is:

$$S_{\mathcal{G}_\mathrm{T}}[\rho(t)] = S_u[\Lambda_{\mathcal{G}_\mathrm{T}}[\rho^E(t)]] = S_u[\Lambda_{\mathcal{G}_\mathrm{T}}[\rho^E_{diag}(t)]]. \tag{4.66}$$

Thus, since the quantum twirling operator $\Lambda_{\mathcal{G}_\mathrm{T}}$ is a unital quantum channel, it follows from the Data Processing Inequality that:

$$D\left[\rho^E_{diag}(t)\|\sigma(t)\right] \geq D\left[\Lambda_{\mathcal{G}_\mathrm{T}}[\rho^E_{diag}(t)]\|\Lambda_{\mathcal{G}_\mathrm{T}}[\sigma(t)]\right] \tag{4.67}$$

for any operator σ where $D[\cdot\|\cdot]$ is the Kullback–Leibler divergence. Therefore, let us take $\sigma = \mathbb{1}$, which leads to the following result, as well as from the definition of the Kullback–Leibler divergence:

$$\begin{aligned} D\left[\rho^E_{diag}(t)\|\sigma(t)\right] &= \operatorname{Tr}\left\{\rho^E_{diag}(t)\log[\rho^E_{diag}(t)] - \rho^E_{diag}(t)\log(\mathbb{1})\right\} \\ &= \operatorname{Tr}\{\rho^E_{diag}(t)\log[\rho^E_{diag}(t)]\} \\ &= -S_d[\rho(t)]. \end{aligned} \tag{4.68}$$

On the other hands, we have:

$$\begin{aligned} D\left[\Lambda_{\mathcal{G}_\mathrm{T}}[\rho^E_{diag}(t)]\|\Lambda_{\mathcal{G}_\mathrm{T}}[\sigma(t)]\right] &= \operatorname{Tr}\left\{\Lambda_{\mathcal{G}_\mathrm{T}}[\rho^E_{diag}(t)]\log[\Lambda_{\mathcal{G}_\mathrm{T}}[\rho^E_{diag}(t)]]\right\} \\ &= -S_{\mathcal{G}_\mathrm{T}}[\rho(t)]. \end{aligned} \tag{4.69}$$

Therefore, from the Data processing inequality in Eq. (4.67), we have:

$$-S_d[\rho(t)] \geq -S_{\mathcal{G}_\mathrm{T}}[\rho(t)] \implies S_d[\rho(t)] \leq S_{\mathcal{G}_\mathrm{T}}[\rho(t)] \tag{4.70}$$

and the property (iii) is proved.

In sequence, we prove the item (iv). We go to construct the therm $S_\Gamma[f_t]$ from $S_{\mathcal{G}_\mathrm{T}}[\rho(t)]$. Let us consider the Hamiltonian H which spectrum has a such number of degeneracies, therefore, we can split the $\mathcal{G}_\mathrm{T}$-entropy as

$$\begin{aligned} S_{\mathcal{G}_\mathrm{T}}[\rho] &= -\operatorname{Tr}\left\{\rho^E_{dd}\log(\rho^E_{dd})\right\} \\ &= -\sum_n (\rho^E_{dd})_{nn}\log[(\rho^E_{dd})_{nn}] \\ &= -\sum_m (\rho^E_{dd})_{mm}\log[(\rho^E_{dd})_{mm}] - \sum_k (\rho^E_{dd})_{kk}\log[(\rho^E_{dd})_{kk}], \end{aligned} \tag{4.71}$$

the labels m and k refer to the average elements of ρ^E associated with the $\mathcal{U}(1)$ group and the $\mathcal{U}(n^k_t > 1)$ group, respectively.

On the other hands, we can split the diagonal entropy such as

$$\begin{aligned} S_d[\rho] &= -\sum_{n=1}^{d}(\rho^E_{nn})\log(\rho^E_{nn}) \\ &= -\sum_m(\rho^E_{mm})\log(\rho^E_{mm}) - \sum_k(\rho^E_{kk})\log(\rho^E_{kk}) \end{aligned} \tag{4.72}$$

Then, substituting Eq.(4.72) into Eq.(4.71), we obtain the following expression:

$$S_{\mathcal{G}_\mathrm{T}}[\rho] = S_d[\rho] + \sum_k(\rho^E_{kk})\log[(\rho^E_{kk})] - \sum_k(\rho^E_{dd})_{kk}\log[(\rho^E_{dd})_{kk}]. \tag{4.73}$$

Now we introduce the functional $S_\Gamma[f_t] = -\operatorname{Tr}\{f_t\log(|f_t|)\}$ and we define f_t, for we have the compact notation, by

$$f_t \equiv \left(\bigoplus_k -\rho^E_{kk}\mathbb{1}_1\right)\bigoplus\left(\bigoplus_k \frac{\operatorname{Tr}\{\rho^E_{n^k_t}\}}{n^k_t}\mathbb{1}_{n^k_t}\right). \tag{4.74}$$

In fact, f_t are a diagonal matrix composed by two diagonal blocks, the first block are associated to all density matrix in energy eigenbasis and the second block we have the average Haar of all density matrix elements associated to groups $\mathcal{U}(n^k_t > 1)$, that is, Eq.(4.74) is the compact form of the equality in Eq.(4.65). Consequently, using the relation Eq. (4.73), the functional $S_\Gamma[f_t]$ and the f_t defined by Eq. (4.74) the equality Eq. (4.64) is obtained.

Now, we prove (v). Indeed, from (iv) we have:

$$S_\Gamma[f_t] = S_{\mathcal{G}_\mathrm{T}}[\rho(t)] - S_d[\rho(t)] \geq 0. \tag{4.75}$$

Since from item (iii) we have that $S_{\mathcal{G}_\mathrm{T}}[\rho(t)] \geq S_d[\rho(t)]$. On the other hand, the cases where the equality holds result directly from Corollary 4.3.1. Thus, all properties are demonstrated as desired. □

First, note that the bound established for gauge entropy in property (iii) also allows us to obtain the following chain of inequalities:

$$0 \leq S_u[\rho(t)] \leq S_d[\rho(t)] \leq S_{\mathcal{G}_T}[\rho(t)] \leq \log(\dim\{\mathcal{H}^d\}), \tag{4.76}$$

where the last inequality follows from the concavity of the Von Neumann entropy functional.

Moreover, note that we constructed the term S_Γ under the assumption that the Hamiltonian has at least one non-degenerate state. However, we can easily extend this result to any possible configuration of degeneracy. To this end, we need to introduce a quantity called the Holevo asymmetry measure, which was initially introduced in the context of finite groups in Ref. [83] and later extended to any Lie groups in Ref. [84]. Thus, let us define it.

Definition 7. *(Holevo asymmetry measure [84]). Let us consider a some group Lie group G which elements are denoted by g and the Haar measure induced by G is $\mathrm{d}\mu$. Then, for any unitary matrices V_g and distribution probability function $p(g)$ the quantity S_Γ defined by:*

$$S_\Gamma \equiv S_u[\Lambda^p_\mu[\rho(t)]] - S_u[\rho(t)], \;\; \Lambda^p_\mu[\rho(t)] \equiv \int \mathrm{d}\mu \, p(g) V_g \rho(t) V_g^\dagger \tag{4.77}$$

is called Holevo asymmetry measure.

Notice that, taking the case where the Haar integral is uniform, that is, $p(g) = 1$, and considering the group G as the thermodynamic group, we can identify S_Γ introduced by Eq.(4.64) as the Holevo asymmetry measure in Eq.(4.77) by inspection, noting that the expression for f_t emerges in the particular case where we have at least one non-degenerate state, whereas the Holevo asymmetry measure always exists.

The Holevo asymmetry measure is an important physical quantity that appears in the context of Information Theory [41, 83, 84, 88]. Physically, S_Γ quantifies the asymmetry present in the original state ρ concerning the group G associated with the quantum twirling operator. Therefore, in the context of the thermodynamic group, the asymmetry of a quantum state is related to how much the diagonal elements of the density operator ρ, in the energy basis, projected onto each subspace $\mathcal{H}_k$ differ from the configuration of maximum randomness in that same subspace $\mathcal{H}_k$.

Furthermore, the introduction of the Holevo asymmetry gives us a new way to evaluate the continuity of the $\mathcal{G}_T$-entropy. In fact, since diagonal entropy is a continuous function, we can then establish a continuity condition for the $\mathcal{G}_T$-entropy by imposing that these entropy's become sufficiently close, thus we have:

$$|S_{\mathcal{G}_T}[\rho(t)] - S_d[\rho(t)]| = S_\Gamma < \epsilon, \; \forall \epsilon > 0 \tag{4.78}$$

Thus, note that the condition for the diagonal entropy to emerge as a particular case of gauge entropy is described in terms of the Holevo asymmetry, with equality reached when S_Γ is arbitrarily small. Also, note that we have already proven the implication that the absence of degeneracies implies equality between gauge and diagonal entropy; however, we have not shown the converse of this statement. In fact, considering states that are not symmetric with respect to the gauge group, we can easily verify this assertion. To this end, let us consider the Data Processing Inequality given by:

$$D\left[\rho(t)\|\sigma(t)\right] \geq D\left[\Lambda_{\mathcal{G}_{\mathrm{T}}}[\rho(t)]\|\Lambda_{\mathcal{G}_{\mathrm{T}}}[\sigma(t)]\right] \tag{4.79}$$

where the equality holds if and only if

$$\rho = \sigma^{1/2}\left(\Lambda_{\mathcal{G}_{\mathrm{T}}}[\sigma(t)]\right)^{-1/2}\left(\Lambda_{\mathcal{G}_{\mathrm{T}}}[\rho(t)]\right)\left(\Lambda_{\mathcal{G}_{\mathrm{T}}}[\sigma(t)]\right)^{-1/2}\sigma^{1/2}. \tag{4.80}$$

Therefore, if $\sigma = \mathbb{1}$, and using the fact of the quantum twirling operator is a unital quantum channel these expressions reduces to:

$$S_{\mathcal{G}_{\mathrm{T}}}[\rho^E_{diag}(t)] = S_u[\rho^E_{diag}] \iff \rho^E_{diag} = \Lambda_{\mathcal{G}_{\mathrm{T}}}[\rho^E_{diag}] \tag{4.81}$$

which is an contradiction, because we suppose that ρ is not invariant state. Then, for states which are not invariant the equality between diagonal and gauge entropy never is achieved. Consequently, the entropy's are equal if and only if the associated thermodynamic group is given by

$$\mathcal{G} = \prod_{k=1}^{d} \mathcal{U}(1)$$

i.e. the case of the Hamiltonian has no degeneracies.

With this, we can then conceive a physical interpretation for gauge entropy. In fact, while diagonal entropy is understood as quantifying the amount of randomness observed in the energy eigenbasis of the system, gauge entropy quantifies this randomness more in relation to the randomness associated with the degeneracy configuration of the Hamiltonian, which appears in the form of the symmetry of the thermodynamic group.

Finally, we will ensure that gauge entropy satisfies the same thermodynamic properties as diagonal entropy [28]. In fact, we can use the operator D to construct the other relation between diagonal and gauge entropy. To do this, let us consider the state $\sigma \equiv D(\rho) = u_t \rho_{dd} u_t^\dagger$; since u_t is not trivially the state, σ is not in the energy eigenbasis, but this state is invariant over the thermodynamic group. Therefore, if we consider the state σ, we can evaluate the diagonal entropy of this state; now note that

$$\sigma_{diag}^{E} = u_t^{\dagger}\sigma u_t = \rho_{dd}^{E} \tag{4.82}$$

therefore the diagonal entropy of σ is:

$$S_d[\sigma] = S_d[\rho_{dd}^{E}] = S_{\mathcal{G}_{\mathrm{T}}}[\rho] \tag{4.83}$$

which implies that: the $\mathcal{G}_{\mathrm{T}}$-entropy can be viewed of the diagonal entropy. This equality implies that the some thermodynamics properties for the diagonal entropy must be valid for the gauge entropy, in special this prove the following relation:

$$\Delta S_{\mathcal{G}_{\mathrm{T}}}[\rho(t)] = S_{\mathcal{G}_{\mathrm{T}}}[\rho(t)] - S_{\mathcal{G}_{\mathrm{T}}}[\rho(0)] \geq 0 \tag{4.84}$$

which describes the gauge entropy production in closed system.

4.3.2 $\mathcal{G}_T$-Entropy and coherent heat

Having established both the expression for gauge entropy and evaluated its properties, we can now explore its relationship with coherent heat. Indeed, starting from Eq. (4.54), we obtain:

$$\begin{aligned}
\frac{d}{dt}S_{\mathcal{G}_{\mathrm{T}}}[\rho(t)] &= -\frac{d}{dt}\,\mathrm{Tr}\left\{\rho_{dd}^{E}\log(\rho_{dd}^{E})\right\}\\
&= -\frac{d}{dt}\,\mathrm{Tr}\left\{\left(\int \mathrm{d}\mathcal{G}_{\mathrm{T}}\, V_t\rho(t)V_t^{\dagger}\right)\log\left(\int \mathrm{d}\mathcal{G}_{\mathrm{T}}{}'\, V_t'\rho(t)V_t'^{\dagger}\right)\right\}\\
&= -\frac{d}{dt}\,\mathrm{Tr}\left\{\rho_{\mathcal{G}}(t)\log(\rho_{\mathcal{G}}(t))\right\}\\
&= -\,\mathrm{Tr}\left\{\frac{d}{dt}\left[\rho_{\mathcal{G}}(t)\right]\log(\rho_{\mathcal{G}}(t)) + \rho_{\mathcal{G}}(t)\rho_{\mathcal{G}}^{-1}(t)\frac{d}{dt}\left[\rho_{\mathcal{G}}(t)\right]\right\}\\
&= -\,\mathrm{Tr}\left\{\frac{d}{dt}\left[\rho_{\mathcal{G}}(t)\right]\log(\rho_{\mathcal{G}}(t))\right\}
\end{aligned} \tag{4.85}$$

where the second term in the penultimate line vanishes due to the density operator's normalization conservation.

From Eq. (4.85) and using the effective density operator dynamics given by Eq. (4.8), we derive:

$$\begin{aligned}
\frac{d}{dt}S_{\mathcal{G}_{\mathrm{T}}}[\rho(t)] &= -\,\mathrm{Tr}\left\{\left(-i\hbar\left[\rho_{\mathcal{G}}(t), H(t)\right] + \mathcal{L}(\rho)\right)\log(\rho_{\mathcal{G}}(t))\right\}\\
&= -\,\mathrm{Tr}\left\{\mathcal{L}(\rho)\log[\rho_{\mathcal{G}}(t)]\right\}.
\end{aligned} \tag{4.86}$$

Equation (4.86) establishes a connection between entropy changes and the non-unitary term of the effective dynamics, which essentially generates the coherent heat energy contribution.

Consequently, this analysis again highlights the irreversible character induced by the coarse-graining through Haar averages.

Nevertheless, the connection between these quantities via the $\mathcal{L}(\rho)$ term already suggests a possible qualitative relationship - first identified through numerical results in Ref. [3] and now theoretically explained in this work.

4.4 Simple aplications

Having obtained the invariant quantities for heat and work as in Ref. [3] and also the $\mathcal{G}_T$-entropy, we will now revisit some of the application examples presented in Ref. [3], which illustrate the applicability of the gauge theory formalism of the thermodynamic group $\mathcal{G}_T$. In particular, the purpose of this section is to present the results shown as examples in Ref. [3] in a pedagogical manner, with the aim of providing the reader with a technical understanding of how the quantities obtained here are calculated. Furthermore, both applications agree with what we discussed in Section 4.2 regarding the behavior of coherent heat and its relation to the production of coherence in a dynamics involving modifications in the energy basis.

4.4.1 Open systems

Let us consider an example presented in Ref.[3] associated with the non-unitary dynamics of a single qubit described by the Hamiltonian $H(t) = g(t)\sigma^z$, where $g(t)$ is a time-dependent function.

While the dynamics are non-unitary, the density operator $\rho(t)$ satisfies the following Lindblad equation:

$$\dot{\rho}(t) = -i\left[H(t), \rho(t)\right] + \mathcal{D}\left[\rho(t)\right], \tag{4.87}$$

with $\mathcal{D}$ being the non-unitary part of the dynamics (dissipator). Furthemore, let us consider the following dissipator:

$$\mathcal{D}_d[\rho] = -\frac{\Gamma_{\text{dec}}}{2}\left[\sigma^z, \left[\sigma^z, \rho\right]\right] \tag{4.88}$$

where σ^z are the $z-$th Pauli matrix, Γ_{dec} represents the decoherence rate $\mathcal{D}_d$ is called the dephasing quantum channel. The second quantum channel is called generalized amplitude damping which is described by the dissipator:

$$\mathcal{D}_a[\rho] =\Gamma_a(\bar{n}+1)\left[\sigma^-\rho\sigma^+ - \frac{1}{2}\left\{\sigma^+\sigma^-, \rho\right\}\right] + \Gamma_a\bar{n}\left[\sigma^+\rho\sigma^- - \frac{1}{2}\left\{\sigma^-\sigma^+, \rho\right\}\right] \tag{4.89}$$

where $\sigma^{\pm}$ are the usual spin ladder operators, $\bar{n} = (e^{-\beta\omega} - 1)^{-1}$ stands for the mean excitation number of the bath mode with frequency ω and β stands for the inverse temperature while Γ_a is the decoherence rate.

Note then that, since the Hamiltonian $H(t)$ is always diagonal, it follows that $H(t)$ is already in its energy basis. By convention, we can diagonalize it so that $h(t) = -g_t\sigma^z$, hence $\dot{h} = -\dot{g}_t\sigma_z$, and in this case, the invariant work is given by:

$$W_{inv}[\rho] = \int_0^{\tau} \mathrm{d}t\, \mathrm{Tr}\left\{-\rho(t)\dot{g}(t)\sigma^z\right\} = \int_0^{\tau} \mathrm{d}t\, \dot{g}(t)\left[\rho_{22}(t) - \rho_{11}(t)\right].$$

On the other hand, since the matrices u_t are time-independent, the coherent heat of the system is zero, indicating that there is no production of coherence in the energy basis. Thus, immediately from equality 4.40, we obtain that the invariant work, in this case, is equal to the usual work, i.e., $W_{inv} = W_u$.

Note that this analysis holds for any dissipator $\mathcal{D}$. In the same vein, we can evaluate the invariant heat, which, in both cases, reduces to the usual heat, i.e., $Q_{inv} = Q_u$. Thus, we obtain:

$$Q_{inv}[\rho] = \int_0^{\tau} \mathrm{d}t\, g(t)\, \mathrm{Tr}\{\sigma^z\mathcal{D}\left[\rho(t)\right]\} = \int_0^{\tau} \mathrm{d}t\, g(t)\left[\left(\mathcal{D}\left[(\rho(t)\right]\right)_{11}\right) - \left(\mathcal{D}\left[\rho(t)\right]\right)_{22}\right].$$

Now, note that in the case where the dissipator is given by Eq. (4.88), we have $Q_{inv} = Q_u = 0$ since all coherence is destroyed by the decoherence process induced by the action of the bath. On the other hand, when the dissipator is given by Eq. (4.89), in addition to the decoherence process, there is also an energy exchange between the system and the bath, which is identified as heat. Integrating the invariant heat identifies the function $\Phi_E(t) \equiv g(t)\left[\left(\mathcal{D}\left[(\rho(t)\right]\right)_{11}\right) - \left(\mathcal{D}\left[\rho(t)\right]\right)_{22}\right]$ associated with the instantaneous energy flow.

This simple example reveals some interesting points about our formalism. First, note that when we have Hamiltonians that are always diagonal, as in the example discussed, we will not have the production of coherence in the energy basis, and thus the expressions obtained for invariant work and heat reduce to the usual notions of quantum thermodynamics presented in Ref. [15]. This ensures consistency with existing developments in the literature [3].

This analysis, along with what we have already discussed in Chapter 3, shows us that the gauge theory of the group $\mathcal{G}_T$ is a theory about how the energy basis of a given Hamiltonian changes over some dynamics. The transitions in the energy basis generate coherence that appears in our description associated with the coherent heat term Q_c.

At the end of this chapter, we will present two examples that were initially explored by Céleri and Rudnicki in Ref. [3], which illustrate this discussion when we have systems where changes occur in the energy basis. In these applications, we will show the connection between coherent heat and the relative entropy of coherences as well as with the notion of invariant entropy that we will introduce in Section 4.3.

4.4.2 Driven single qubit

Consider the problem of a single qubit in a guided magnetic field, which is driven by a protocol $g(t)$ and is described by the following time-dependent Hamiltonian:

$$H = \sigma^z + g(t)\sigma^x = \begin{pmatrix} 1 & g(t) \\ g(t) & -1 \end{pmatrix} \tag{4.90}$$

where σ^z and σ^x are the Pauli matrices associated with the z and x components, respectively. In fact, this Hamiltonian is a very special case of the Landau-Zener model [47, 92–94]. Specifically, here $g(t)$ is a smooth continuous time-dependent function that describes the controlled injection or extraction of energy in the system. In this sense, this system is closed, and the evolution of the density matrix follows the Liouville-Von Neumann Eq. (2.21); therefore, the usual heat is zero, i.e., $Q_u[\rho] = 0$.

Our goal will be to obtain expressions for the invariant heat and work. In fact, let us start by obtaining the eigenvalues $\lambda(t)$, which can be easily obtained from Eq. (4.90), given by:

$$\lambda_{\pm}(t) = \pm\lambda, \;\; \lambda \equiv \sqrt{1 + g(t)^2}. \tag{4.91}$$

Furthermore, the normalized eigenvectors associated with each eigenvalue are given by:

$$|a_0(t)\rangle = \begin{pmatrix} -\dfrac{g(t)}{\sqrt{2\lambda(\lambda+1)}} \\ \\ \dfrac{1+\lambda(t)}{\sqrt{2\lambda(\lambda+1)}} \end{pmatrix}, \; |a_1(t)\rangle = \begin{pmatrix} \dfrac{1+\lambda}{\sqrt{2\lambda(\lambda+1)}} \\ \\ \dfrac{g(t)}{\sqrt{2\lambda(\lambda+1)}} \end{pmatrix}, \tag{4.92}$$

and consequently, the matrix u_t associated with the energy basis of the Hamiltonian in Eq. (4.90) is given by:

$$u_t = \begin{pmatrix} -\dfrac{g(t)}{\sqrt{2\lambda(\lambda+1)}} & \dfrac{1+\lambda}{\sqrt{2\lambda(\lambda+1)}} \\ \\ \dfrac{1+\lambda(t)}{\sqrt{2\lambda(\lambda+1)}} & \dfrac{g(t)}{\sqrt{2\lambda(\lambda+1)}} \end{pmatrix}. \tag{4.93}$$

Since the set$\{|a_0(t)\rangle, |a_1(t)\rangle\}$ is orthonormal basis, the following relations hold:

$$\begin{cases} \langle \dot{a}_0(t)|a_1(t)\rangle = -\langle a_0(t)|\dot{a}_1(t)\rangle = \dfrac{\dot{g}(t)}{2\lambda^2}, \\ \langle \dot{a}_0(t)|a_0(t)\rangle = \langle \dot{a}_1(t)|a_1(t)\rangle = 0 \end{cases}. \tag{4.94}$$

With this, we can already obtain the expressions for invariant work and coherent heat. Indeed, using Eq. (4.45), we obtain that the invariant work is given by:

$$W_{inv}[\rho(t)] = \int_0^\tau \mathrm{d}t \sum_{n=0}^{1} \rho^E_{n,n}(t)\dot{\lambda}_n(t) = \int_0^\tau \mathrm{d}t\, \frac{g(t)\left(\rho^E_{11}(t) - \rho^E_{00}(t)\right)}{\sqrt{1+g^2(t)}}. \tag{4.95}$$

On the other hand, the coherent heat is easily obtained using Eq. (4.46), which gives us that:

$$\begin{aligned} Q_c[\rho(t)] &= \int_0^\tau \mathrm{d}t \sum_{n,m=0}^{1} \rho^E_{mn}(t) \langle \dot{a}_n(t)|a_m(t)\rangle \left(\lambda_m(t) - \lambda_n(t)\right) \\ &= \int_0^\tau \mathrm{d}t\, \rho_{01}(t)\frac{\dot{g}(t)}{2\lambda^2}\cdot(-2\lambda) - \rho_{10}(t)\frac{\dot{g}(t)}{2\lambda^2}\cdot(2\lambda) \\ &= 2\int_0^\tau \mathrm{d}t\, \mathrm{Re}[\rho^E_{01}(t)]\frac{\dot{g}(t)}{\sqrt{1+g(t)^2}}. \end{aligned} \tag{4.96}$$

Finally, note that both Eq. (4.95) and Eq. (4.96) depend on the coefficients of the density operator. To obtain these terms, we must solve the Liouville-Von Neumann equation considering the Hamiltonian given in Eq. (4.90). In this sense, we must have, considering the operators in the energy basis:

$$\begin{aligned} \frac{\mathrm{d}\,\rho^E}{\mathrm{d}t} &= -i[h, \rho^E] \\ &= -i\left[\sum_{n,m=0}^{1} \lambda_n(t)\rho^E_{nm}(t)\left|a_n\right\rangle\left\langle a_m\right| - \sum_{n,j=0}^{1} \rho^E_{jn}(t)\lambda_n(t)\left|a_j\right\rangle\left\langle a_n\right|\right] \\ &= -i\left[\lambda_0\rho^E_{00}\left|a_0\right\rangle\left\langle a_0\right| + \lambda_0\rho^E_{01}\left|a_0\right\rangle\left\langle a_1\right| + \lambda_1\rho^E_{10}\left|a_1\right\rangle\left\langle a_0\right| + \lambda_1\rho^E_{11}\left|a_1\right\rangle\left\langle a_1\right|\right] + \\ &+ i\left[\rho^E_{00}\lambda_0\left|a_0\right\rangle\left\langle a_0\right| + \rho^E_{10}\lambda_0\left|a_1\right\rangle\left\langle a_0\right| + \rho^E_{01}\lambda_1\left|a_0\right\rangle\left\langle a_1\right| + \rho^E_{11}\lambda_1\left|a_1\right\rangle\left\langle a_1\right|\right] \\ &= -i\left[\left(\lambda_0\rho^E_{01} - \lambda_1\rho^E_{01}\right)\left|a_0\right\rangle\left\langle a_1\right| + \left(\lambda_1\rho^E_{01} - \lambda_0\rho^E_{10}\right)\left|a_1\right\rangle\left\langle a_0\right|\right] \\ &= -2i\lambda_0\left[\rho^E_{01}\left|a_0\right\rangle\left\langle a_1\right| - \rho^E_{10}\left|a_1\right\rangle\left\langle a_0\right|\right]. \end{aligned} \tag{4.97}$$

On the other hands, we can expand the derivative of $\rho^E(t)$ as:

$$\begin{aligned} \frac{\mathrm{d}\,\rho^E}{\mathrm{d}t} &= \frac{\mathrm{d}}{\mathrm{d}t}\left(\sum_{j,k=0}^{1} \rho^E_{j,k}\left|a_j\right\rangle\left\langle a_k\right|\right) \\ &= \sum_{j,k=0}^{1} \dot{\rho}^E_{j,k}\left|a_j\right\rangle\left\langle a_k\right| + \dot{\rho}^E_{j,k}\left|\dot{a}_j\right\rangle\left\langle a_k\right| + \dot{\rho}^E_{j,k}\left|a_j\right\rangle\left\langle \dot{a}_k\right| \\ &= \dot{\rho}_{00}\left|a_0\right\rangle\left\langle a_0\right| + \dot{\rho}_{10}\left|a_1\right\rangle\left\langle a_0\right| + \dot{\rho}_{01}\left|a_0\right\rangle\left\langle a_1\right| + \dot{\rho}_{11}\left|a_1\right\rangle\left\langle a_1\right| + \\ &+ \rho_{00}\left|\dot{a}_0\right\rangle\left\langle a_0\right| + \rho_{10}\left|\dot{a}_1\right\rangle\left\langle a_0\right| + \rho_{01}\left|\dot{a}_0\right\rangle\left\langle a_1\right| + \rho_{11}\left|\dot{a}_1\right\rangle\left\langle a_1\right| + \\ &+ \rho_{00}\left|a_0\right\rangle\left\langle \dot{a}_0\right| + \rho_{10}\left|a_1\right\rangle\left\langle \dot{a}_0\right| + \rho_{01}\left|a_0\right\rangle\left\langle \dot{a}_1\right| + \rho_{11}\left|a_1\right\rangle\left\langle \dot{a}_1\right|. \end{aligned} \tag{4.98}$$

Given the equalities between Eq. (4.97) and Eq. (4.98) and using the relationships between the eigenstates $|a_0\rangle$ and $|a_1\rangle$ expressed in Eq. (1), we can obtain the following set of ordinary differential equations:

$$\begin{cases} \dot{\rho}^E_{11} = -\dfrac{\dot{g}(t)}{2\lambda^2}\left(\rho^E_{12} + \rho^E_{21}\right) \\ \dot{\rho}^E_{12} = 2i\lambda\rho^E_{12} + \dfrac{\dot{g}(t)}{2\lambda^2}\left(\rho^E_{11} - \rho^E_{22}\right) \\ \dot{\rho}^E_{21} = -2i\lambda\rho^E_{21} - \dfrac{\dot{g}(t)}{2\lambda^2}\left(\rho^E_{22} - \rho^E_{11}\right) \\ \dot{\rho}^E_{22} = \dfrac{\dot{g}(t)}{2\lambda^2}\left(\rho^E_{12} + \rho^E_{21}\right). \end{cases} \tag{4.99}$$

The system displayed in Eq. (4.99) is not analytically integrable. However, with an initial condition in hand, the system in Eq. (4.99) can be easily solved numerically.

Then, in order to retrieve the results developed by Céleri and Rudnicki in Ref. [3], let us choose $g(t) = \cos(t)$. Regarding the $\mathcal{G}_T$-entropy, note that the eigenvalues are given by Eq. (4.91), and since g^2 is always positive, it follows that $\lambda_0(t) \leq \lambda_1(t)$ for every instant of time t, meaning that the system is non-degenerate. Consequently, the $\mathcal{G}_T$-entropy reduces to diagonal entropy, as shown in the previous section.

Thus, by choosing the initial state as the ground state of the Hamiltonian in Eq. (4.90), i.e., $\rho(0) = |a_0(t=0)\rangle\langle a_0(t=0)|$, we manage to obtain the invariant heat and work as well as the coherence entropy Eq. (2.59), which we present in Figure 4.1.

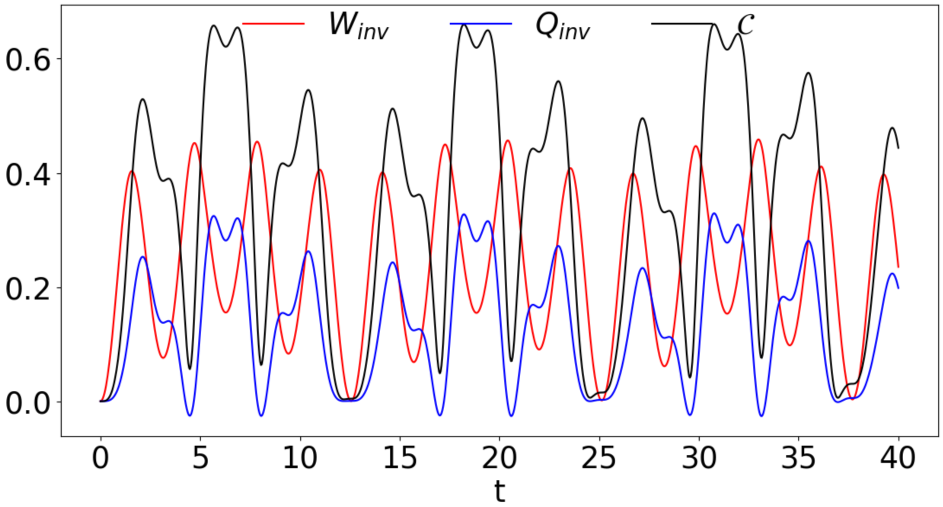

FIGURE 4.1: Invariant work, Invariant Heat and Coherence for single qubit with drive in Hamiltonian in Eq. (4.90).

Unlike the example we presented in Section 4.2, this example contrasts with what we expect from usual quantum thermodynamics when assuming unitary evolution [17, 95, 96]. However, this result is perfectly consistent with the definitions of heat introduced in closed systems for quantum adiabatic processes [22, 24, 28]. Our findings establish a strong physical foundation – the gauge theory of the thermodynamic group $\mathcal{G}_T$ – for understanding the link between heat in closed quantum systems and energy delocalization. This principle explains the oscillatory behavior of heat during closed evolution, where coherences fluctuate over time.

4.4.3 Driven spin chains

The Landau-Zener model described by the Hamiltonian in Eq. (4.90) presents certain inherent difficulties in the formalism. In particular, these difficulties emerge when we think about how to generalize the previous development to many-body systems, which are particularly relevant in the context of quantum thermodynamics [47, 97, 98]. However, we often find ourselves relying on numerical methods due to the impossibility of an analytic treatment of certain systems. Indeed, one of the difficulties we encounter is in evaluating the coherent heat, given the need to obtain the derivatives of the matrices u_t. However, at least in the context of closed systems, we can simplify this process through the first law of thermodynamics.

In this sense, we will show a practical approach to addressing the problem associated with determining the invariant heat and work. To this end, we will consider Hamiltonians of the form:

$$H(t) = H_0 + g(t)H_1 \tag{4.100}$$

where $g(t)$ is the control protocol associated with the coherent injection of energy into the system. Moreover, H_0 and H_1 are two Hermitian operators that may or may not commute with each other.

Now, let us consider that we have an initial state prepared at $t \leq 0$, given by $\rho(0)$. It follows that if $\rho(0)$ is some pure state, then the temporal evolution can be obtained by solving the Schrödinger equation with $H(t)$ using some numerical method. If $\rho(0)$ is a thermal state, its evolution is then determined by the solution of the Liouville-Von Neumann equation.

Thus, as $H(t)$ is given by Eq. (4.100), we can obtain that the derivative of the system's energy is given by:

$$\frac{\mathrm{d}\,\mathrm{U}[\rho(t)]}{\mathrm{dt}} = \frac{\mathrm{d}}{\mathrm{dt}}\operatorname{Tr}\{\rho H\} = \operatorname{Tr}\left\{\rho\frac{\mathrm{d}}{\mathrm{dt}}\left[H_0 + g(t)H_1\right]\right\} = \frac{\mathrm{d}\,g(t)}{\mathrm{dt}}\operatorname{Tr}\{\rho H_1\}. \tag{4.101}$$

On the other hand, the derivative of the energy also gives us the following development:

$$\begin{aligned}\frac{\mathrm{d}\,\mathrm{U}[\rho(t)]}{\mathrm{dt}} &= \frac{\mathrm{d}}{\mathrm{dt}}\mathrm{Tr}\left\{\rho H\right\} \\ &= \mathrm{Tr}\left\{\rho(t)\frac{\mathrm{d}}{\mathrm{dt}}(u_t h u_t^\dagger)\right\} \\ &= \mathrm{Tr}\left\{\rho\left(\dot{u}_t h u_t^\dagger + u_t h \dot{u}_t^\dagger\right)\right\} + \mathrm{Tr}\left\{\rho(u_t \dot{h}_t u_t^\dagger)\right\} \\ &= \frac{\mathrm{d}}{\mathrm{dt}}\left[\int_0^\tau dt\,\mathrm{Tr}\left\{\rho\left(\dot{u}_t h u_t^\dagger + u_t h \dot{u}_t^\dagger\right)\right\} + \mathrm{Tr}\left\{\rho(u_t \dot{h}_t u_t^\dagger)\right\}\right] \\ &= \frac{\mathrm{d}\,Q_c[\rho(t)]}{\mathrm{dt}} + \frac{\mathrm{d}\,W_{inv}[\rho](t)}{\mathrm{dt}}. \end{aligned} \tag{4.102}$$

With Eqs. (4.101) and Eq. (4.102) at hand, we can obtain the coherent heat in an alternative way, which is then given by:

$$\frac{\mathrm{d}\,Q_c[\rho(t)]}{\mathrm{dt}} = \frac{\mathrm{d}\,\mathrm{U}[\rho(t)]}{\mathrm{dt}} - \frac{\mathrm{d}\,W_{inv}[\rho(t)]}{\mathrm{dt}}. \tag{4.103}$$

Thus, the problem for the case where the system dynamics is unitary can be expressed by the following set of equations.

$$\begin{cases} W_{inv}[\rho(t)] = \displaystyle\int_0^\tau \mathrm{dt}\,\mathrm{Tr}\left\{\rho^E(t)\frac{\mathrm{d}\,h(t)}{\mathrm{dt}}\right\} \\ \dfrac{\mathrm{d}\,\mathrm{U}[\rho(t)]}{dt} = \dfrac{\mathrm{d}\,g(t)}{\mathrm{dt}}\mathrm{Tr}\left\{\rho(t)H_1\right\} \\ \dfrac{\mathrm{d}\,Q_c[\rho(t)]}{\mathrm{dt}} = \dfrac{\mathrm{d}\,\mathrm{U}[\rho(t)]}{\mathrm{dt}} - \dfrac{\mathrm{d}\,W_{inv}[\rho(t)]}{\mathrm{dt}} \end{cases} . \tag{4.104}$$

In this sense, we will apply this technique to study the unitary dynamics of the following Hamiltonian:

$$H(t) = -\frac{k}{2j}J_x^2 - g(t)J_z \tag{4.105}$$

where $J_\alpha = \sum_{i=1}^{N}\sigma_i^\alpha/2$; $(\alpha = x, y, z)$ are the collective spin operators, with σ_i^α denoting the α Pauli matrix acting on the i-th site of a chain of $N = 2j$ sites, and j is the total angular momentum.

The Hamiltonian presented in Equation Eq. (4.105) represents a specific case of the widely recognized Lipkin-Meshkov-Glick (LMG) model, as detailed in references [99–101]. The LMG model has been extensively investigated in various fields, including nuclear physics [102], optics [103], quantum information [104], and condensed matter physics [105], among others.

In particular, the Lipkin-Meshkov-Glick (LMG) model is relevant to our context due to the existence of degenerate energy levels for certain values of the magnetic field $g(t)$. In particular, for $g < k$, the energy levels are doubly degenerate, while for $g > k$, the Hamiltonian in Eq. (4.105) exhibits no degeneracies in the thermodynamic limit [104, 106]. Indeed, at this moment we are only interested in obtaining a model that can serve as a platform to test our formalism; therefore, we have no particular interest in effects associated with the model, such as quantum phase transitions, which we will explore in the following chapter.

For simplicity, let us consider $k = 1$, and the function associated with the magnetic field will be given by: $g(t) = \beta \tanh(\alpha t)$. The choice of the hyperbolic tangent function as a protocol is strategic [3], as the parameters α and β allow us to control the speed and amplitude of the protocol, respectively. For arbitrarily large values of α, i.e. $\alpha \to \infty$, the dynamics of the Hamiltonian operator tends toward a sudden quench; on the other hand, when we take the opposite limit, i.e., $\alpha \to 0$, we obtain the case of very slow driving.

For the LMG model, as with the previous model, we need to solve the time-dependent Schrödinger equation. In this sense, we have two paths to follow. The first path consists of writing the state $|\psi\rangle$ as:

$$|\psi(t)\rangle = \sum_{m=-j}^{j} f_m(t)\, |j, m\rangle \tag{4.106}$$

where we expand the state in the angular momentum basis $\{|j, m\rangle\}$ with time-dependent coefficients $f_m(t)$. Then, substituting the above state into the Schrödinger equation and taking the inner product with the bra $\langle j, n|$, we obtain the following development:

$$\begin{aligned}
i\frac{d}{dt}\langle j, n|\psi(t)\rangle &= -\frac{k}{2j}\langle j, n|J_x^2\, |\psi(t)\rangle\rangle - g(t)\langle j, n|J_z\, |\psi(t)\rangle\rangle \\
&= -\frac{k}{2j}\langle j, n|\frac{J_+^2 + J_-^2 + \{J_+, J_-\}}{4}|\psi\rangle - g(t) n f_n(t) \\
&= -\frac{k}{8j}\left[\langle j, n|J_-^2|\psi\rangle + \langle j, n|J_+^2|\psi\rangle + \langle j, n|\{J_+, J_-\}|\psi\rangle\right] - g(t) n f_n(t) \\
&= -\frac{k}{8j}\Big[\sqrt{(j+n+2)(j-n-1)(j+n+1)(j-n)} f_{n+2}(t) + \\
&+ \sqrt{(j-n+2)(j+n-1)(j-n+1)(j+n)} f_{n-2}(t) + 2(j(j+1) - n^2) f_n(t)\Big] \\
&- g(t) n f_n(t).
\end{aligned}$$

Therefore, we obtain the following expression:

$$\begin{aligned}
i\dot{f}_n(t) &= -\frac{k}{8j}\Big[\sqrt{(j+n+2)(j-n-1)(j+n+1)(j-n)} f_{n+2}(t) \\
&+ \sqrt{(j-n+2)(j+n-1)(j-n+1)(j+n)} f_{n-2}(t)\Big] - \left[\frac{(j(j+1) - n^2)}{4j} + n g(t)\right] f_n(t),
\end{aligned} \tag{4.107}$$

which defines a recursive expression for the coefficients $f_n(t)$ of the state $\psi(t)$ as $2j+1$ linear first-order differential equations. Thus, studying the time-dependent dynamics of the LMG model can be done using the above expression and implementing a suitable numerical method for its solution. Indeed, it is worth noting that the implementation of numerical methods such as fourth- or fifth-order Runge-Kutta for solving the above system is valid; however, this is only efficient for low values of j. In fact, since it is interesting to study the dynamics of the system for large values of j to approach the thermodynamic limit, these numerical methods become somewhat imprecise, and their convergence is affected. This can be compensated for by excessively increasing the time step, leading to a significant increase in computation time. With this in mind, this approach is not very efficient. However, a way to circumvent this issue is by using the ‘mesolve‘ method from the QuTiP framework [107], which, through adaptive methods, can handle these high-dimensional systems with good accuracy.

In Figure 4.2, we can see the distinction between the $\mathcal{G}_T$-entropy and diagonal entropy for various values of amplitude intensity β.

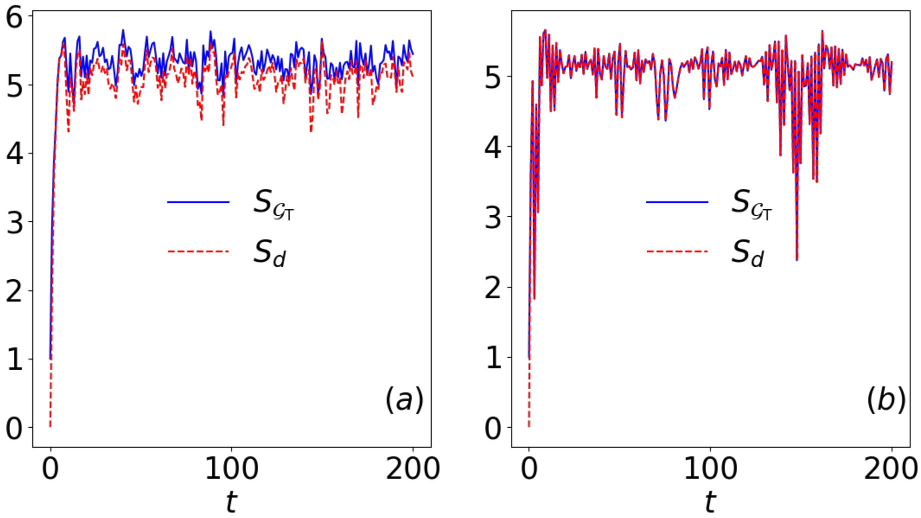

FIGURE 4.2: $\mathcal{G}_T$-entropy and diagonal entropy as functions of time for the ground state of the Hamiltonian (4.105) at $t = 0$ as a function of time, with the amplitude parameter $\beta = 0.5$ and $\beta = 1.5$ respectively in figures (a) and (b). We choose $j = 50$ and $\alpha = 1$ for all curves.

As expected, figure Eq. (4.2) exemplifies the result we showed in Ineq. (4.63), thus highlighting the increase of entropy in degenerate systems. Next, in Figure 4.3, we obtained the behavior of the $\mathcal{G}_T$-entropy for different values of the protocol speed α. The coherent heat under the same conditions as Figure 4.3 is shown in Figure 4.4. As expected, the behavior obtained for the coherent heat in Figure 4.4 agrees with the way the $\mathcal{G}_T$-entropy scales, as well as with the findings in Ref. [3].

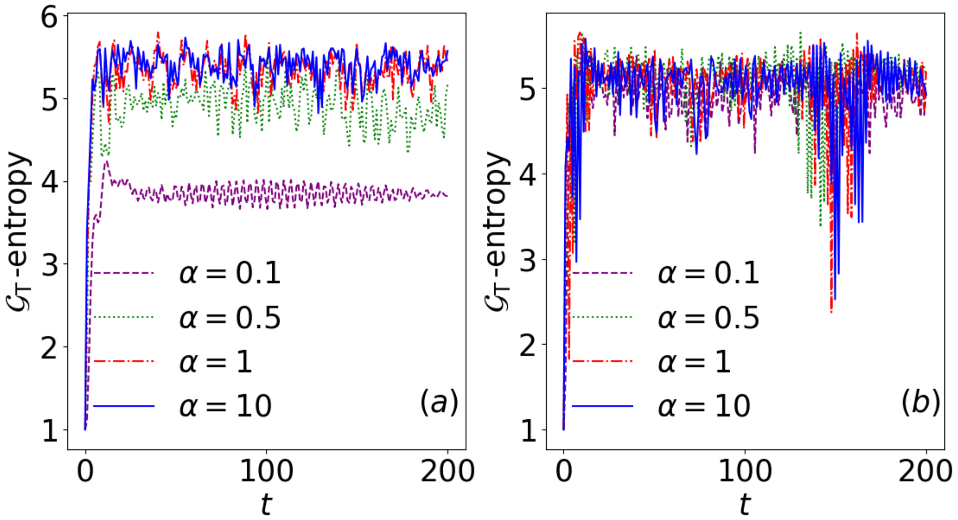

FIGURE 4.3: Behavior of the gauge entropy for the evolution of the ground state of the Hamiltonian (4.105) at $t = 0$ for $\beta = 0.5$ in (a) and $\beta = 1.5$ in (b) for different values of the speed of the protocol α. We choose $j = 50$ for all curves.

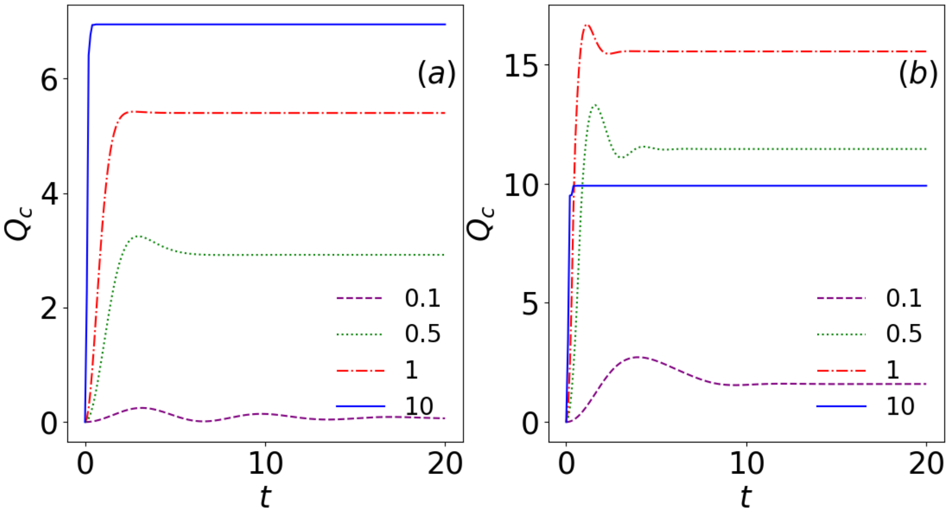

FIGURE 4.4: Coherent heat for the LMG model. The initial state is the ground state of the Hamiltonian (4.105) at $t = 0$ for $\beta = 0.5$ in (a) and $\beta = 1.5$ in (b), for distinct values of the speed of the protocol α. We choose $j = 50$ for all curves.

This example shows how the coherent heat scales with the generation of coherences. Over time, we shift from an adiabatic Hamiltonian transformation (which is too slow to generate coherences) to a regime where coherences are created. This transition is accompanied by an increase in heat generation. In this regime, rapid changes in the Hamiltonian inevitably induce transitions between energy eigenstates, and these transitions are associated with heat production.

Chapter 5

Gauge approach to thermodynamics of critical systems

In this chapter we will introduce a novel approach to the study of quantum critical systems under the view of gauge invariant quantum thermodynamics.

Since the thermodynamics of the critical systems are the main focus of this chapter, we will start the first section of this chapter with a brief overview of the quantum phase transition. The following sections of this chapter constitutes the original development in the gauge-invariant quantum thermodynamics. In this sense, we introduce the specific derivation of the expressions for the invariant work and heat associated to the quench dynamics.

Finally, we will apply this formalism to study the quantum phase transition of two different spin models: Landau-Zener model and Lipkin-Meshkov-Glick model.

5.1 Quantum phase transition

In the context of classical physics, phase transitions are a type of critical phenomenon that involve changes in the macroscopic properties of a system. Particularly in equilibrium thermodynamics, a phase change occurs when a certain parameter, usually temperature, reaches a critical value at which certain thermodynamic quantities exhibit non-analytic behavior, thereby marking the phase transition [5]. In this context, a classic example is the liquid-solid phase transition of water, which occurs when the temperature decreases to the critical temperature of $T_c = 273.15°K$. Beyond this value, the macroscopic structure of water shifts to the solid phase. During this process, as water solidifies into ice, both the specific volume and the thermodynamic entropy of the system become discontinuous, which is the non-analyticity that marks this phase transition [5, 108].

The liquid-solid phase transition of water is just one of the various examples of phase transitions that occur in classical systems. Other examples include magnetic systems, which may exhibit transitions between ferromagnetic and paramagnetic phases, other simple fluids like water, as well as fluid mixtures [108]. A precise understanding of this phenomenon was achieved through statistical mechanics, more specifically by the modern techniques introduced by the renormalization group [108, 109].

However, prior to the establishment of the renormalization group formalism, several theories, generally phenomenological, were developed to provide explanations for the phase transition phenomenon, with particular emphasis on Landau's phenomenological theory.

Landau's phenomenological description introduced new elements and concepts for understanding phase transitions. In particular, his theory involved developing an expansion of the Gibbs free energy functional f in terms of a function $\eta \equiv \eta(g)$, which is called the order parameter, defined as follows:

$$\begin{cases} \eta(g) \neq 0 \text{ if } g < g_c \\ \eta(g) = 0 \text{ if } g > g_c \end{cases} . \tag{5.1}$$

The argument (g) corresponds to the physical quantity that drives the phase transition; in the classical context, g generally represents temperature. Moreover, the value g_c in Eq. (5.1) is known as the critical point, which marks the phase transition that occurs between the ordered phase $g < g_c$ and the disordered phase $g > g_c$. Along with the existence of order parameters, Landau's theory also predicted the existence of critical exponents, which describe how certain physical quantities behave throughout a phase transition.

Furthermore, Landau's theory, based on the order parameter in Eq. (5.1), allows for the classification of a phase transition into two types. The first type is the first-order phase transition, characterized by an abrupt change in the order parameter η; consequently, Landau's functional f shows a discontinuity at the critical point g_c . On the other hand, when the higher than second order derivatives of the functional f exhibit discontinuity, the phase transition is said to be of second order.

Indeed, the advances brought by these concepts were truly significant in understanding phase transitions, even though these initial definitions were not sufficient to explain phase transitions in general. However, the introduction of the renormalization group through the works of Kenneth G. Wilson [110–112] provided an explanation for the phase transition phenomenon. In particular, the renormalization group made it possible to calculate the critical exponents, which were not precisely calculable within Landau's phenomenological framework [108].

So far, we have discussed aspects associated with phase transitions that occur in classical systems, which are generally driven by temperature. However, phase transitions can also be observed beyond the classical limit, particularly in the context of quantum systems [113].

Indeed, in quantum systems at ($T = 0$), we can observe quantum phase transitions (QPT), which, unlike classical phase transitions, are not driven by temperature but rather by some control parameter g associated with the Hamiltonian of the system. However, note that at $T = 0$, the

Gibbs free energy reduces to the ground state energy, and consequently, statistical averages are replaced by ground state averages. Thus, the quantum phases of the system become characterized by the ground state.

With this in mind, let us consider a Hamiltonian $H(g)$ that depends on a dimensionless coupling parameter g. In essence, we are interested in Hamiltonians of the following type:

$$H(g) = H_0 + gH_1, \tag{5.2}$$

where H_0 and H_1 are two arbitrary observables. Notice that if H_0 and H_1 commute, i.e., $[H_0, H_1] = 0$, then there exists a common basis in which H_0 and H_1 can be simultaneously diagonalized. On the other hand, if these operators do not commute, i.e., $[H_0, H_1] \neq 0$, it is not possible to diagonalize them simultaneously. Consequently, the non-commutativity of the operators H_0 and H_1 implies that the ground state and eigenenergy of the Hamiltonian $H(g)$ are expressed as functions of the coupling parameter g.

In this sense, the presence of the operator H_1 in a system initially described by H_0 introduces quantum fluctuations that are controlled by the coupling parameter g. Indeed, the strength of the coupling g establishes a competitive relationship between the operators H_0 and H_1 that make up the Hamiltonian, such that, for $g \ll 1$, the system is dominated by H_0, whereas for $g \gg 1$, the system tends to be dominated by the contributions of H_1. Therefore, since the parameter g can be continuously modified, there must exist a critical value g_c such that the energy gap Δ between the ground state and the first excited state is minimized, resulting in a singularity in the ground state for $g = g_c$.

In this context, the critical value g_c is called the quantum critical point (QCP), analogous to the critical point introduced in the context of classical phase transitions. Thus, as the system approaches the thermodynamic limit, the gap Δ might close, and a singularity may develop in the ground state and ground state energy [113]. In the context of the QPT, this constitutes a continuous quantum phase transition. Especially as the system approaches the QCP, both for $g < g_c$ and $g > g_c$

$$\Delta \sim K \left| g - g_c \right|^{z\nu}, \tag{5.3}$$

where z and ν are the dynamic and correlation length critical exponents and K is the energy scale of characteristic microscopic coupling. In fact, the relation (5.3) can be made formal by a mapping between the partition function of a d-dimensional quantum system and a $(d+1)$-dimensional classical system [113–115]. This mapping associates the inverse of the quantum energy gap with a diverging correlation length in the classical model's "time" direction. This correlation length diverges with an exponent.

In this sense, let us observe the behavior of the partition function Z in the limit as T approaches zero. Indeed, let the partition function be given by:

$$Z(\beta) = \mathrm{Tr}\{e^{-\beta H}\}, \tag{5.4}$$

where H is the Hamiltonian and $\beta \equiv (k_B T)^{-1}$. In fact, we can reconstruct all thermodynamic quantities from Z. Notice that we can identify the operator $e^{-\beta H}$ equivalently as the time evolution operator including the time interval $\tau = \hbar\beta$, therefore:

$$e^{-\beta H} \to U(\tau) \equiv e^{-(\tau/\hbar)H}, \ \tau = \hbar\beta, \tag{5.5}$$

where operator $U(\tau)$ is the imaginary-time propagator. This operator is equivalent to the time evolution operator $e^{-iHt/\hbar}$, if we identify the time interval t with the imaginary value $t = -i\hbar\beta$.

Since the mapping in Equation (5.5) is a rotation associated with the time interval τ, we can obtain subintervals of time $\delta\tau$, such that

$$e^{-\beta H} \to U(\tau) \equiv e^{-(\tau/\hbar)H} = \left(e^{-(\delta\tau/\hbar)H}\right)^N \tag{5.6}$$

where $\delta\tau$ is an imaginary time interval that is small on the relevant time scales, and N is a large integer such that $N\delta\tau = \hbar\beta$.

So when we write the partition function as

$$\begin{aligned} Z(\beta) &= \sum_n \langle n| e^{-\beta H} |n\rangle = \sum_n \langle n| e^{-(\tau/\hbar)H} |n\rangle \qquad (5.7) \\ &= \sum_n \langle n| e^{-(\delta\tau/\hbar)H} |n\rangle \\ &= \sum_n \sum_{m_1,\ldots,m_N} \langle n| e^{-(\delta\tau/\hbar)H} |m_1\rangle \langle m_1| e^{-(\delta\tau/\hbar)H} |m_2\rangle \ldots \langle m_N| e^{-(\delta\tau/\hbar)H} |n\rangle \qquad (5.8) \end{aligned}$$

where in (5.8) we introduced the complete and orthogonal set $\{|m_i\rangle\}_{i=1,\ldots,N}$ for every factor in the expression of $Z(\beta)$.

First, note that in Eq. (5.7), the partition function Z is the sum of transition amplitudes associated with the imaginary time the system returns to the same state after an imaginary time $t = -i\tau$. The thermodynamic properties of a quantum system are inextricably linked to its dynamics in imaginary time, a departure from the classical statistical mechanics framework.

In classical systems, dynamics and thermodynamics can be treated as independent entities, with the position and momentum variables in the partition function being mutually independent. However, the non-commutativity of position and momentum operators in quantum mechanics necessitates a unified approach to dynamics and thermodynamics, resulting in a more elaborate treatment.

The expression of the quantum partition function in Eq. (5.8) has the same form resembles a classical partition function formulated using a transfer matrix $\mathbf{T}$, since we indentify $\mathbf{T}$ with $e^{-\delta\tau H/\hbar}$. This implies that the imaginary time dimension in the quantum system can be interpreted as an extra spatial dimension in a classical system. Consequently, a d-dimensional quantum system will exhibit a partition function analogous to that of a classical system in $(d+1)$ dimensions.

However, this extra spatial dimension has a finite extent, being limited by $\hbar\beta = \hbar(k_B T)^{-1}$ in units of time. Therefore, as $T \to 0$, the size of the additional spatial dimension diverges, and the dual classical system becomes fully $(d+1)$-dimensional.

This result provides us with an elegant connection between a quantum system that is d-dimensional and a $(d+1)$-dimensional classical system when $T = 0$. In this sense, we may expect to be able to describe quantum phase transitions using the same tools as for classical phase transitions. In particular, since diverging correlation lengths are a generic feature of classical continuous phase transitions [113], this implies diverging correlation length ξ and correlation time ξ_τ at the continuous quantum phase transition (QPT), since both are effective correlation lengths in a dual classical system. We also expect that as the system approaches the quantum critical point by letting the parameter g move towards g_c, they will diverge according to some critical exponents.

$$\xi \quad \sim K\left|g-g_c\right|^{-\nu} \text{ and } \xi_\tau \quad \sim \xi^z. \tag{5.9}$$

Then, utilizing the relations in Eq.(5.9), we arrive at the result stated in Eq.(5.3) for the characteristic energy scale Δ, which is defined by the energy gap to the lowest excitation above the ground state. In this sense, the energy scale Δ can be related as the lenght scale by

$$\Delta \sim \xi^{-z} \sim K|g-g_c|^{z\nu} \tag{5.10}$$

when $g \to g_c$.

For the case of $T = 0$, a schematic representation of the phase diagram for a quantum phase transition is shown in Figure 5.1.

In fact, the quantum phase transition are characterized by the null temperature. However, a quantum phase transition (QPT) can also occur at non-zero temperatures. [113, 115], In particular, it can occur even in systems at high temperatures. [47, 97].

Indeed, let L_τ be the size of the extra spatial dimension given by $\hbar\beta$. As we consider $T > 0$, the size of the extra dimension L_τ decreases. Thus, if g is far enough from the quantum critical point g_c such that the correlation time ξ_τ is less than L_τ, the non-zero temperature does not affect the behavior of the system. Consequently, the system is fully quantum, as thermal fluctuations

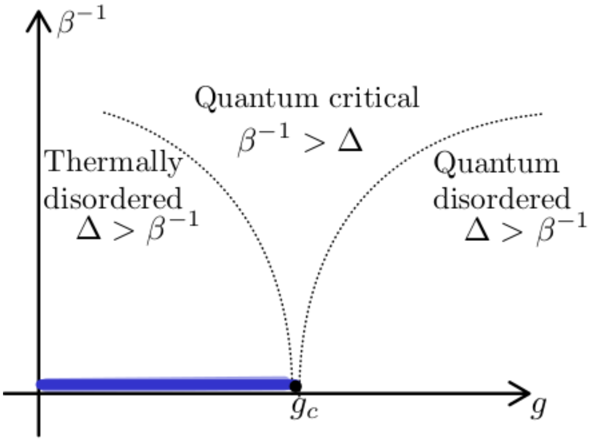

FIGURE 5.1: Schematic representation of a diagram of quantum phase transition at $T = 0$. The ordered phase exists only at $T = 0$ and below the quantum critical point g_c, which is represented by the blue line. Above the quantum critical point lies a region loosely bounded by $T \sim |g - g_c|^{z\nu}$, where the temperature scaling can be observed. This figure was created by the author, inspired by the illustrations in Ref. [113].

cannot excite the ground states since the energy scale of the thermal fluctuations is always smaller than the energy scale associated with the gap of the quantum system, that is, $\Delta > \beta^{-1}$.

On the other hand, as $g \to g_c$, the correlation time will be such that $\xi_\tau > \hbar\beta$. Therefore, unlike the case when $T = 0$, the d-dimensional quantum system will be mapped to a d-dimensional classical system. In this case, quantum phase transitions can still occur, being present in a region called "quantum critical," see Figure 5.2, which is characterized by $\beta^{-1} > \Delta$, where the energy scales of the thermal fluctuations at the critical point are greater than the energy scale of the gap between the ground state. In the quantum critical region, once we have $\beta^{-1} > \Delta$, the thermal

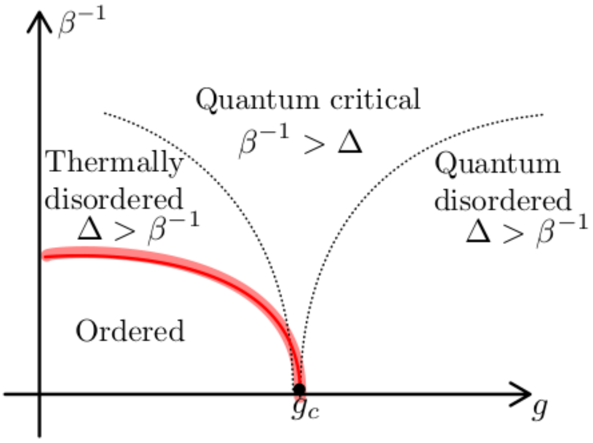

FIGURE 5.2: Schematic representation of a diagram of quantum phase transition at $T \neq 0$. A line of finite temperature critical points, indicated in red, ends at the quantum critical point. The shaded area surrounding this line is where classical critical phenomena are observed. This figure was created by the author, inspired by the illustrations in Ref. [113].

energies are capable of exciting the ground state. Consequently, the physical behavior of the thermal excitations is governed by the quantum critical point [113]. In this case, both thermal and quantum fluctuations play equally significant roles in the quantum phase transition. Furthermore, the system cannot be treated as a classical system but rather by a continuous quantum field theory.

5.2 QPT in gauge $\mathcal{G}_{\mathrm{T}}$-theory

Critical effects, in particular, quantum phase transitions, are especially interesting in the context of quantum thermodynamics. The criticality associated with these transitions can induce significant effects, such as the production of entropy and the generation of quantum coherence [47, 61, 97]. In this sense, work protocols have proven to be valuable tools for investigating criticalities, especially in quenches during quantum phase transitions (QPTs).

In a quench, the control parameter of a system is rapidly varied, driving the system through a quantum critical point, where its fundamental properties change abruptly. By monitoring the evolution of the work done during this process, it is possible to identify signatures of criticality, such as the closing of the energy gap and the increase in work fluctuations [95, 116].

These protocols allow for the quantification of the average work and work distributions [95]. These are sensitive to changes in the characteristics of the system, such as the presence of low-energy excitations and the non-equilibrium dynamics induced by the quench [95, 117].

In this sense, we construct a specific protocol for study quantum phase transitions in gauge invariant quantum thermodynamics. For this, we construct a specific Hamiltonian inspired in the quench protocol [95]. Indeed, let us consider the following general Hamiltonian:

$$H_\alpha(t) = H_0 + [g_0 + \delta g f_\alpha(t)]H_1, \quad f_\alpha(t) = \frac{1}{2} + \frac{1}{2}\tanh(\alpha(t-\tau)). \tag{5.11}$$

Here, H_0 and H_1 are two Hermitian operators that generally do not commute, i.e., $[H_0, H_1] \neq 0$, and both are time-independent. Furthermore, g_0 is a fixed parameter in the Hamiltonian, and the protocol is defined by the function $f_\alpha(t)$, which modifies the Hamiltonian over time in such a way that from a given instant $t = \tau$, the Hamiltonian smoothly changes so that the total coupling associated with the operator H_1 changes from g_0 to $g = g_0 + \delta g$. In Figure 5.3, we plot the protocol function $f_\alpha(t)$ for different values of the speed α.

The choice of the protocol given by the function $f_\alpha(t)$ allows us to control, smoothly, the modification of the Hamiltonian $H_\alpha(t)$. In particular, the limiting case of high velocities, that is, $\alpha \to \infty$, is extremely relevant for our objective of constructing a mathematical description analogous to a quench. Indeed, in the high-velocity regime, we can obtain the following relations

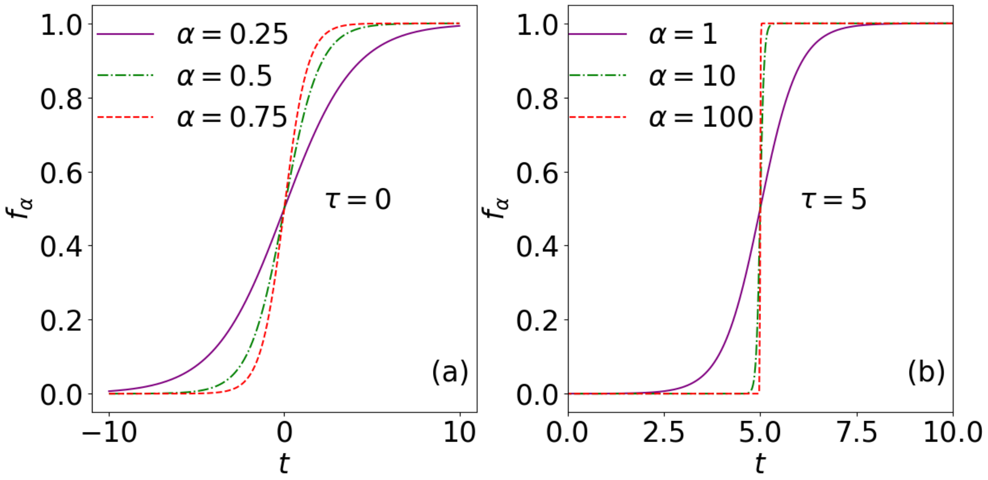

FIGURE 5.3: Representation of the protocol function $f_\alpha(t)$ for different values of α, we use $\tau = 0$ and $\tau = 5$ respectively in the panels (a) and (b).

for the function $f_\alpha(t)$:

$$\begin{cases} \lim\limits_{\alpha\to\infty} f_\alpha(t) = \lim\limits_{\alpha\to\infty} \left[\frac{1}{2} + \frac{1}{2}\tanh(\alpha(t-\tau))\right] = \theta(t-\tau), \\ \\ \lim\limits_{\alpha\to\infty} \frac{\mathrm{d}[f_\alpha(t)]}{\mathrm{dt}} = \lim\limits_{\alpha\to\infty} \left[\frac{\alpha}{2}\,\mathrm{sech}^2(\alpha(t-\tau))\right] = \delta(t-\tau), \end{cases} \tag{5.12}$$

where $\theta(t-\tau)$ and $\delta(t-\tau)$ are the Heaveside function and delta Dirac distribution respectively, which are defined as:

- The Heaviside function is a simple unit step function defined by:

$$\theta(t-\tau) = \begin{cases} 0, & \text{if } t < \tau, \\ 1, & \text{if } t \geq \tau. \end{cases} \tag{5.13}$$

- Delta Dirac distribution are characterized by:

$$\int_E \mathrm{dt}\,\delta(t-\tau)\phi(t) = \phi(\tau) \text{ and } \int_E \mathrm{dt}\,\delta(t-\tau) = 1 \tag{5.14}$$

  where $E \subset \mathbb{R}$ is any interval of the line centered at τ, and $\phi(t)$ is an arbitrary test function, i.e., $\phi \in C_c^\infty$.

In fact, the second equality—for the limit of $\frac{\mathrm{d}\,f_\alpha}{\mathrm{dt}}$—in Eq. (1) is also valid in the sense of distributions. Furthermore, the relevant properties can be found in any standard text on mathematical physics, such as [55, 118, 119], or even in more advanced treatments of functional analysis and the theory of distributions, such as [120, 121].

[1]

Proceeding with our objective, let us then evaluate the work associated with the protocol described by the Hamiltonian given by Eq (5.11). Indeed, we have:

$$W_u[\rho(t)] = \int_0^{t_f} \mathrm{dt}\, \mathrm{Tr}\left\{\rho(t)\frac{\mathrm{d}(H_\alpha(t))}{\mathrm{dt}}\right\} = \int_0^{t_f} \mathrm{dt}\, \mathrm{Tr}\left\{\rho(t)\delta g H_1\right\} \frac{\mathrm{d}\, f_\alpha(t)}{\mathrm{dt}} \tag{5.16}$$

where the protocol occurs in $t \in [0, t_f]$. Specifically, we are interested in the case where the protocol occurs rapidly enough that it corresponds to taking the limit as $\alpha \to \infty$. Furthermore, the dynamics in a quench protocol must be such that at $t = 0$, the initial state evolves under the action of the post-quench Hamiltonian; that is, in addition to enforcing the limit for high velocities of the protocol, we must use that $t_f = \tau + \epsilon$, where τ and ϵ are arbitrarily small. Indeed, by applying these conditions to Eq. (5.16), we obtain the following development:

$$\begin{aligned} W_{u,\infty}[\rho(t)] &\equiv \lim_{\alpha\to\infty} W_u[\rho(t) \qquad (5.17)\\ &= \lim_{\alpha\to\infty} \int_0^{\tau+\epsilon} \mathrm{dt}\, \mathrm{Tr}\left\{\rho(t)\delta g H_1\right\} \frac{\mathrm{d}\, f_\alpha(t)}{\mathrm{dt}} \\ &= \int_0^{\tau+\epsilon} \mathrm{dt}\, \mathrm{Tr}\left\{\rho(t)\delta g H_1\right\} \delta(t-\tau) \qquad (5.18)\\ &= \frac{1}{2}\, \mathrm{Tr}\left\{\rho(\tau)\delta g H_1\right\}, \qquad (5.19) \end{aligned}$$

in which, in Eq. (5.18), we use the distributional convergence of the protocol function $f_\alpha(t)$ to the Dirac delta distribution. Finally, we evaluate the integral and obtain Eq. (5.19), which is the work performed by the system with the protocol function $f_\alpha(t)$ in the rapid velocity limit.

Moreover, in this same limit of the protocol function $f_\alpha(t)$, we have that:

$$H_\alpha(t) \to H_g(t), \text{ where } H_g(t) = H_0 + [g_0 + \delta g \theta(t-\tau)]H_1, \tag{5.20}$$

---

[1] For a critical reader, we provide further details regarding the precise use of the Dirac delta function. Specifically, we define the one-dimensional Dirac delta function, δ, as a linear functional on the Sobolev space $W^{1,p}(\Omega) = \{f \in L^p(\Omega \subset \mathbb{R}) \mid f' \in L^p$, where f' denotes the weak derivative of $f\}$, mapping to the field $\mathbb{K} = \mathbb{R}$ or $\mathbb{C}$. That is, we consider $\delta : W^{1,p} \to \mathbb{K}$, where, for every $f \in W^{1,p}(\Omega)$, we have the distributional equality

$$\langle f, \delta\rangle_{L^p(\Omega\subset\mathbb{R})} = f(0). \tag{5.15}$$

Thus, the Dirac delta function is defined as an element of the dual space of $W^{1,p}(\Omega)$, which is precisely the Sobolev space $W_0^{-1,p}(\Omega)$.

From a functional analysis perspective, in Sobolev spaces, classical notions of continuity and differentiation are replaced by concepts of "almost everywhere" continuity and weak derivatives. Consequently, operations involving the Dirac delta function become well-posed in the distributional sense. More precisely, the weak formulation ensures that differentiation extends naturally to distributions, and elements of $W_0^{-1,p}(\Omega)$ can be interpreted as continuous linear functionals acting on $W^{1,p}(\Omega)$. This approach not only legitimizes the use of the delta function in rigorous mathematical settings but also aligns with the broader framework of Sobolev embedding theorems and duality principles in functional spaces.

since $\alpha \to \infty$ and, therefore, for $t = \tau$ we have: $\delta g H_1 = H_g - H_{g_0}$ where $H_{g_0} \equiv H_0 + g_0 H_1$. Using this, we can write the following equalities:

$$W_{u,\infty}[\rho(t)] = \frac{1}{2}\operatorname{Tr}\{\rho(\tau)\delta g H_1\} = \frac{1}{2}\operatorname{Tr}\{\rho(\tau)H_g - \rho(\tau)H_{g_0}\}. \tag{5.21}$$

Therefore, the expression (5.21) gives us two equalities for the work, defined in the Alicki sense, for this protocol.

Then, since we have the expression for this protocol, we can define invariant work and heat in quenches. Firstly, we introduce the notion of invariant work to the quench limit for $f_\alpha(t)$ dynamics by the following theorem:

Theorem 5. *(Gauge-Invariant work for quench). Let the Hamiltonian defined in (5.11), where H_0 and H_1 may or may not commute. Then, the invariant work associated with a quench limit for $f_\alpha(t)$ dynamics of arbitrary amplitude δg are given by:*

$$W_{inv}[\rho_t] \;=\; \frac{1}{2}\operatorname{Tr}\left\{\rho^E_{diag}(\tau)H_g(\tau) - \rho^E_{dd}(\tau)H_{g_0}(\tau)\right\} \tag{5.22}$$

where ρ^E_{dd} is given by (3.42) in instant $t = \tau$. If the Hamiltonian as not degenerate energy level the expression (5.22) reduces to:

$$W_{inv}[\rho] = \frac{1}{2}\operatorname{Tr}\left\{(H_g - H_{g_0})\,\rho^E_{diag}(\tau)\right\}. \tag{5.23}$$

Proof. Using Eq. (5.19) and the Definition 3 we have:

$$\begin{aligned}
W_{inv}\,[\rho] &= \int d\mathcal{G}_{\mathrm{T}}\, W_{u,\infty}[V_t\rho(t)V_t^\dagger] \\
&= \int d\mathcal{G}_{\mathrm{T}}\, \frac{1}{2}\operatorname{Tr}\left\{V_\tau\rho(\tau)V_\tau^\dagger[H_g - H_{g_0}]\right\} \\
&= \frac{1}{2}\operatorname{Tr}\{\rho(\tau)H_g\} - \frac{1}{2}\operatorname{Tr}\left\{\int d\mathcal{G}_{\mathrm{T}}\left(V_\tau\rho(\tau)V_\tau^\dagger\right)H_{g_0}\right\} \\
&= \frac{1}{2}\operatorname{Tr}\{\rho(\tau)H_g\} - \frac{1}{2}\operatorname{Tr}\left\{\Lambda_{\mathcal{G}_{\mathrm{T}}}[\rho^E(\tau)]H_{g_0}\right\} \\
&= \frac{1}{2}\operatorname{Tr}\left\{\rho^E_{diag}(\tau)H_g - \rho^E_{dd}(\tau)H_{g_0}\right\}
\end{aligned}$$

where the superscript E, here, denote the energy eigenbasis in instant τ, i.e. $X^E = u_\tau^\dagger X u_\tau$ for some matrix X and ρ^E_{dd} are given in Eq. (3.42).

In the particular case where the Hamiltonian exhibits no degeneracy in its energy levels, i.e. $n_1 = n_2 = \ldots = n_d = 1$, therefore:

$$\rho^E_{dd}(\tau) = \bigoplus_{k=1}^{d} \frac{\operatorname{Tr}\left\{\rho^E_{n_k}(\tau)\right\}}{1}\mathbb{1}_1 = \rho^E_{diag}(\tau)$$

which is the density operator with the off-diagonal (in the the energy eigenbasis) elements removed. Then, the expression for the invariant work in this case follow as:

$$W_{inv}[\rho] = \frac{1}{2}\operatorname{Tr}\left\{(H_g - H_{g0})\,\rho^{E}_{diag}(\tau)\right\}$$

as wished. $\square$

On the other hands, the expression of invariant heat is easy obtained from the First Law of Thermodynamics.

Furthermore, in the same spirit of the Chapter 4, we going to obtain the expression for the invariant heat. Indeed, this quantity is presented in the following Theorem.

Theorem 6. *(Gauge-Invariant heat for quenches). Under the same assumptions of Theorem 5. Then, the notion of invariant heat is given by*

$$Q_{inv}[\rho] = Q_u[\rho] + Q_c[\rho], \tag{5.24}$$

where

$$Q_c[\rho] = \frac{1}{2}\operatorname{Tr}\left\{\left(\rho^{E}_{dd}(\tau) - \rho^{E}(\tau)\right) H_{g0}\right\}. \tag{5.25}$$

Proof. This proof is simple, considering the regime of high speed of the protocol function $f_\alpha(t)$ and using the Definition 3 we have the following development:

$$\begin{aligned}
Q_{inv}\left[\rho\right] &= \int \mathrm{d}\mathcal{G}_{\mathrm{T}}\, Q_u\left[V_t\rho V_t^{\dagger}\right] \\
&= \int \mathrm{d}\mathcal{G}_{\mathrm{T}} \int_0^{\tau} \mathrm{dt}\,\operatorname{Tr}\left\{H(t)\frac{\mathrm{d}}{\mathrm{dt}}\left(V_t\rho V_t^{\dagger}\right)\right\} \\
&= Q_u[\rho] + \int \mathrm{d}\mathcal{G}_{\mathrm{T}} \int_0^{\tau} \mathrm{dt}\,\operatorname{Tr}\left\{H(t)\left(\frac{\mathrm{d}\,V_t}{\mathrm{dt}}\rho V_t^{\dagger} + V_t\rho\frac{\mathrm{d}\,V_t^{\dagger}}{\mathrm{dt}}\right)\right\} \\
&+ \int \mathrm{d}\mathcal{G}_{\mathrm{T}} \int_0^{\tau} \mathrm{dt}\,\operatorname{Tr}\left\{V_t\rho V_t^{\dagger}\frac{\mathrm{d}\,H(t)}{\mathrm{dt}} - V_t\rho V_t^{\dagger}\frac{\mathrm{d}\,H(t)}{\mathrm{dt}}\right\} \\
&= Q_u[\rho] + \int \mathrm{d}\mathcal{G}_{\mathrm{T}} \int_0^{\tau} \mathrm{dt}\,\operatorname{Tr}\left\{\rho\frac{\mathrm{d}}{\mathrm{dt}}(V_tH(t)V_t^{\dagger})\right\} - W_{inv}[\rho] \\
&= Q_u[\rho] + W_{u,\infty}[\rho] - W_{inv}[\rho] \\
&= Q_u[\rho] + \frac{1}{2}\operatorname{Tr}\left\{\rho(\tau)H_g(\tau) - \rho(\tau)H_{g0}\right\} - \frac{1}{2}\operatorname{Tr}\left\{\rho(\tau)H_g(\tau) - \rho^{E}_{dd}H_{g0}\right\} \\
&= Q_u[\rho] + \frac{1}{2}\operatorname{Tr}\left\{\left(\rho^{E}_{dd} - \rho^{E}\right) H_{g0},\right\},
\end{aligned}$$

where we using the commuting relation between the Hamiltonian and the gauge transformation i.e. $[V_t, H] = 0$. Then, defining:

$$Q_c[\rho] \equiv \frac{1}{2}\,\mathrm{Tr}\left\{\left(\rho^E_{dd} - \rho^E\right) H_0,\right\}$$

we have the desired. □

Before we proceed with the discussions on the invariant heat and work obtained for a quench process, note that we can rewrite the expressions for both functionals. Indeed, using Eq. (5.19), we can obtain the invariant work through the following development:

$$\begin{aligned} W_{inv}[\rho] &= \int \mathrm{d}\mathcal{G}_{\mathrm{T}}\, \frac{\delta g}{2}\, \mathrm{Tr}\{V_\tau \rho(\tau) V_\tau^\dagger H_1\} \\ &= \frac{\delta g}{2}\, \mathrm{Tr}\left\{\int \mathrm{d}\mathcal{G}_{\mathrm{T}}\, V_\tau \rho(\tau) V_\tau^\dagger H_1\right\} \\ &= \frac{\delta g}{2}\, \mathrm{Tr}\{\rho^E_{dd}(\tau) H_1\}. \end{aligned} \tag{5.26}$$

Similarly, the coherent heat can be rewritten; in fact, starting from the development made in the proof of Theorem 6, we have:

$$\begin{aligned} Q_{inv}[\rho] &= Q_u[\rho] + W_{u,\infty}[\rho] - W_{inv}[\rho] \\ &= Q_u[\rho] + \frac{1}{2}\,\mathrm{Tr}\left\{\rho(\tau)\delta g H_1\right\} - \frac{\delta g}{2}\,\mathrm{Tr}\{\rho^E_{dd}(\tau) H_1\} \\ &= Q_u[\rho] + \frac{\delta g}{2}\,\mathrm{Tr}\left\{\left(\rho^E(\tau) - \rho^E_{dd}(\tau)\right) H_1,\right\}, \end{aligned} \tag{5.27}$$

which identifies the coherent heat as:

$$Q_c[\rho] = \frac{\delta g}{2}\,\mathrm{Tr}\left\{\left(\rho^E(\tau) - \rho^E_{dd}(\tau)\right) H_1\right\}. \tag{5.28}$$

Note that the development from the Hamiltonian (5.11) becomes equivalent to the development arising from the high-velocity limit obtained by taking $\alpha \to \infty$, as given in Eq. (5.20). In this sense, the problem of treating a Hamiltonian as given in Eq. (5.2) involves constructing a time-dependent counterpart as in Eq. (5.11). Subsequently, all the results we obtained are analogous.

5.2.1 Physical meaning of invariant heat and work in the QPT framework

Now, just as we did in Chapter 4, we will discuss a bit about the physical meaning of the expressions associated with the invariant heat and work obtained from Theorem 5 and Theorem 6, as well as the equivalent expressions obtained in Eq. (5.26) and Eq. (5.28).

In fact, the expressions for invariant heat and work obtained in this section follow the same spirit as the quantities obtained by Céleri and Rudnicki in Ref. [3] and reproduced in Chapter 4. From a purely mathematical perspective, the results of Theorem 5 and Theorem 6 relax the differentiability hypothesis of the energy basis u_t, thus allowing a new class of physical processes associated with abrupt and instantaneous modifications within the framework of the thermodynamic group $\mathcal{G}_{\mathrm{T}}$. For this reason, the physical meaning associated with these quantities, as discussed in Chapter 4, must also be extended.

Indeed, the physical interpretation of invariant work and coherent heat as, respectively, effective work and heat associated with information access limitations about the system remains valid. As previously discussed in this section, we can mathematically develop these expressions using test function sequences in distribution spaces, allowing us to achieve the desired equalities in a distributional sense that naturally extends to the classical notion of continuity we are familiar with. This analysis is particularly relevant for the derivation of the dynamical equation initially obtained in Eq. (4.8).

With this technical caveat established, let us proceed to analyze the physical meaning of these quantities. As mentioned, given the validity of Eq. (4.8), even in cases of abrupt Hamiltonian changes $H(t)$, the physical interpretation remains intact. However, what changes here is that due to the nature of the control parameter $g(t)$, jump terms appear in both heat and work expressions, explicitly associated with populations that originate from the thermodynamic group structure.

From Eq. (5.25) and writing $\rho^E(\tau) = \rho^E_{diag}(\tau) + \rho^E_c(\tau)$, where $\rho^E_{diag}(\tau)$ and $\rho^E_c(\tau)$ represent the diagonal (populations) and off-diagonal (coherences) parts of the density operator in the energy basis, we obtain:

$$Q_c[\rho] = \frac{1}{2}\operatorname{Tr}\left\{(\rho^E_{dd} - \rho^E)H_{g_0}\right\} = \frac{1}{2}\operatorname{Tr}\left\{(\rho^E_{dd} - \rho^E_{diag})H_{g_0}\right\} - \frac{1}{2}\operatorname{Tr}\left\{\rho^E_c H_{g_0}\right\}. \tag{5.29}$$

The first term in Eq. (5.29) contains population contributions that emerge when Hamiltonian spectrum degeneracies exist. Notably, when degeneracies are absent or removed (i.e., $\rho^E_{dd}(\tau) = \rho^E_{diag}(\tau)$), Eq. (5.29) reduces to:

$$Q_c[\rho] = \frac{1}{2}\operatorname{Tr}\left\{\left(\rho^E_{diag} - \rho^E_{diag}\right)H_{g_0}\right\} - \frac{1}{2}\operatorname{Tr}\left\{\rho^E_c H_{g_0}\right\} = -\frac{1}{2}\operatorname{Tr}\left\{\rho^E_c H_{g_0}\right\} \tag{5.30}$$

recovering the result previously obtained in Eq. (4.46) for Q_c.

This contribution to coherent heat arises from the relative difference between populations of the ρ^E_{dd} state obtained through thermodynamic group coarse-graining and the diagonal part of the density operator, both in the energy basis. However, the purely diagonal state can still be associated with the gauge group when no degeneracies are present. Thus, the first term in Eq. (5.29) can be interpreted as a relative difference between states obtained via coarse-graining with an arbitrary thermodynamic group versus one without degeneracies.

The coarse-graining procedure not only treats coherences as heat but also interprets degeneracy structure as heat. This is naturally expected since energy spectrum degeneracies induce greater randomness in system configurations. In our framework, this randomness emerges as an energy quantity corresponding to the first term in Eq. (2.63), which represents uncontrollable energy and is therefore interpreted as heat.

This result aligns with the relation between gauge entropy and coherent heat in Eq. (4.86), mediated by the heat generator term $\mathcal{L}(\rho)$ in the effective dynamics. This equation reveals that coherent heat and gauge entropy are fundamentally connected, and as we've shown, the entropy can be explicitly decomposed into diagonal entropy plus the Holevo asymmetry (Eq. (4.77)), which has non-zero contribution if and only if the Hamiltonian spectrum is non-degenerate. Consequently, Hamiltonian degeneracies translate to thermodynamic group asymmetry, causing both entropic increase and additional heat contributions.

Furthermore, we can establish a mathematical connection between invariant work and coherent heat with the average work associated with quench processes (stemming from stochastic work definitions) [23, 92]:

$$2W_{inv}[\rho] = \langle W \rangle - 2Q_c[\rho], \tag{5.31}$$

which bears striking resemblance to Eq. (4.40) obtained for continuous processes. This reinforces the interpretation of invariant work and coherent heat, including all sign-dependent analyses discussed in Chapter 4.

Here we also identify the so-called "inner friction" [23] - an energy contribution associated with non-equilibrium processes often treated as closed-system irreversibility. However, the authors in [23] do not clearly classify inner friction as either work or heat, despite suggesting its typical association with heat. Within our formalism, we identify coherent heat as analogous to inner friction, but with a well-defined physical interpretation as heat (not work or some form of "friction"[2]).

The invariant work, conversely, depends entirely on populations and energy level differences induced by Hamiltonian modifications. This result strongly supports our approach, particularly the framework developed in Chapter 4, while maintaining consistency with classical heat/work notions that inspired our formalism.

Having made this discussion, we will now proceed with the application of this formalism to two spin systems, one without degeneracy and the other with degeneracy.

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[2] The friction analogy attempts to connect this quantity with classical physics concepts. However, classically dissipated friction energy emerges from electromagnetic interactions rather than intrinsic quantum effects. This terminology introduces ambiguity for quantum-defined quantities, particularly those connected to energy basis changes - a concept absent in classical physics.

5.3 QPT in Landau-Zener model

Let us consider the dynamics of a single qubit described by the following Hamiltonian

$$H_{LZ}(t) = \left(-\frac{\Delta}{2} + ag\right)\sigma^z + \epsilon\sigma^x, \tag{5.32}$$

where σ^x and σ^z are Pauli matrices, and g stands for the strength of the externally controlled magnetic field, whose coupling with the qubit is represented by $a > 0$. ϵ is associated with the crossing ($\epsilon = 0$) or non-crossing ($\epsilon > 0$) energy levels and Δ is the bare frequency of the qubit.

Hamiltonian Eq. (5.32) is the well-known Landau-Zener model, which is frequently employed in studies of phase transitions as it is a prototype for critical systems [92, 97]. The system undergoes a quantum phase transition at the critical point $g_c = \Delta/2a$ and $\epsilon \to 0$. For $\epsilon > 0$, the transition is a first-order one, characterised by a discontinuous change in the order parameter. When $\epsilon = 0$, the transition becomes a second-order one, exhibiting a continuous change in the order parameter and associated critical fluctuations. A schematic representation of these situations is presented in Fig. 5.4.

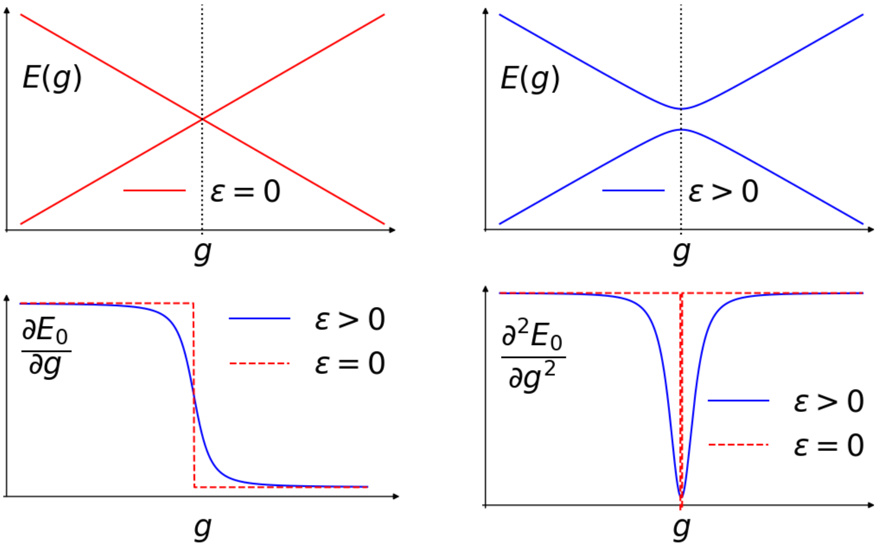

FIGURE 5.4: Schematic representation of the eigenenergies of the Landau-Zener Hamiltonian with and without energy crossing and the rate of variation of the ground state energy with respect to the control parameter g.

Based on the Hamiltonian (5.11), the time dependent version of Eq. (5.32) can be construct, resulting in

$$H_{LZ}(t) = \left(-\frac{\Delta}{2} + a(g_0 + \delta g\theta(t-\tau))\right)\sigma^z + \epsilon\sigma^x. \tag{5.33}$$

In this way, $H_{g_0} = (-\Delta/2 + ag_0)\,\sigma^z + \epsilon\sigma^x$ and $H_1 = a\sigma^z$. It is straightforward to compute both the invariant work and heat associated to this quench.

First, we define, for simplicity, $\gamma_0 \equiv -\Delta/2 + ag_0$. For $t \geq \tau$, the Hamiltonian of the Landau-Zener model is given by Eq. (5.33), which can be exactly diagonalized resulting in the eigenvalues $E_{0,1}(g_0) = \pm E = \pm\sqrt{(a\delta g + \gamma_0)^2 + \epsilon^2}$ and respective normalized eigenvectors

$$|a_0^g\rangle = \begin{pmatrix} -\dfrac{\epsilon}{\sqrt{\phi^2+\epsilon^2}} \\ \dfrac{\phi}{\sqrt{\phi^2+\epsilon^2}} \end{pmatrix}, \; |a_1^g\rangle = \begin{pmatrix} \dfrac{\phi}{\sqrt{\phi^2+\epsilon^2}} \\ \dfrac{\epsilon}{\sqrt{\phi^2+\epsilon^2}} \end{pmatrix} \tag{5.34}$$

where $\phi \equiv \left(\sqrt{(a\delta g + \gamma_0)^2 + \epsilon^2} + a\delta g + \gamma_0\right)$ and $g = g_0 + \delta g$.

In each process with $g_0 \to g_0 + \delta g$, the initial Hamiltonian of the system is

$$H_{g_0} = (-\Delta/2 + ag_0)\,\sigma^z + \epsilon\sigma^x$$

and we take the initial state of the system as $\rho \equiv \rho(0) = |a_0^{g_0}\rangle\langle a_0^{g_0}|$, that is

$$\rho = \begin{pmatrix} \dfrac{1}{2} - \dfrac{\gamma_0}{2\sqrt{\gamma_0^2+\epsilon^2}} & -\dfrac{\epsilon}{2\sqrt{\gamma_0^2+\epsilon^2}} \\ -\dfrac{\epsilon}{2\sqrt{\gamma_0^2+\epsilon^2}} & \dfrac{1}{2} + \dfrac{\gamma_0}{2\sqrt{\gamma_0^2+\epsilon^2}} \end{pmatrix}, \tag{5.35}$$

In the energy eigenbasis, we have ρ^E transformed by the unitary matrix defined by $|a_0^g\rangle$ and $|a_1^g\rangle$. Its elements in this basis are given by

$$\begin{cases} \rho_{11}^E = \dfrac{\sqrt{\gamma_0^2+\epsilon^2}\sqrt{(a\delta g+\gamma_0)^2+\epsilon^2} + a\delta g\gamma_0 + \gamma_0^2 + \epsilon^2}{2\sqrt{\gamma_0^2+\epsilon^2}\sqrt{(a\delta g+\gamma_0)^2+\epsilon^2}} \\ \\ \rho_{12}^E = \rho_{21}^E = -\dfrac{a\delta g\epsilon}{2\sqrt{\gamma_0^2+\epsilon^2}\sqrt{(a\delta g+\gamma_0)^2+\epsilon^2}} \\ \\ \rho_{22}^E = \dfrac{\sqrt{\gamma_0^2+\epsilon^2}\sqrt{(a\delta g+\gamma_0)^2+\epsilon^2} - \gamma_0(a\delta g+\gamma_0) - \epsilon^2}{2\sqrt{\gamma_0^2+\epsilon^2}\sqrt{(a\delta g+\gamma_0)^2+\epsilon^2}} \end{cases}. \tag{5.36}$$

The operator ρ_{diag}^E is given by the diagonal matrix whose elements are $(\rho_{diag}^E)_{jj} = (\rho_0^E)_{jj}$ and $(\rho_{\text{diag}}^E)_{jk} = 0$. Similarly, the coherent density matrix in energy eigenbasis ρ_c is defined by $(\rho_c^E)_{jk} = (\rho_0^E)_{jk}$ and $(\rho_c^E)_{jj} = 0$.

Now, we need to transform each Hamiltonian to the energy basis for $t \geq \tau$. Since $H(\tau)$ in this basis is simply the diagonal matrix with its eigenvalues E_0 and E_1, we only need to obtain the representation of H_0, which is given by

$$H_0^E = \begin{pmatrix} -\dfrac{a\delta g\gamma_0 + \gamma_0^2 + \epsilon^2}{\sqrt{(a\delta g + \gamma_0)^2 + \epsilon^2}} & \dfrac{a\delta g\epsilon}{\sqrt{(a\delta g + \gamma_0)^2 + \epsilon^2}} \\ \\ \dfrac{a\delta g\epsilon}{\sqrt{(a\delta g + \gamma_0)^2 + \epsilon^2}} & \dfrac{a\delta g\gamma_0 + \gamma_0^2 + \epsilon^2}{\sqrt{(a\delta g + \gamma_0)^2 + \epsilon^2}} \end{pmatrix}.$$

We can now compute the invariant work and heat. Making it term by term, we have

$$\mathrm{Tr}\left\{\rho_{diag}^E H_0^E\right\} = -\frac{\left(a\delta g\gamma_0 + \gamma_0^2 + \epsilon^2\right)^2}{\sqrt{\gamma_0^2 + \epsilon^2}\left((a\delta g + \gamma_0)^2 + \epsilon^2\right)} \tag{5.37}$$

$$\mathrm{Tr}\left\{\rho_{diag}^E H^E\right\} = -\frac{a\delta g\gamma_0 + \gamma_0^2 + \epsilon^2}{\sqrt{m^2 + \epsilon^2}} \tag{5.38}$$

$$\mathrm{Tr}\{\rho_c^E H_0^E\} = -\frac{a^2 g^2 \epsilon^2}{\sqrt{\gamma_0^2 + \epsilon^2}\left((ag + \gamma_0)^2 + \epsilon^2\right)}. \tag{5.39}$$

Using these expressions, we can immediately obtain the following expressions for invariant work and heat. In fact, the invariant work is given by:

$$W_{inv}[\rho] = -\frac{a\delta g(a\delta g + \gamma_0)\left(a\delta g\gamma_0 + \gamma_0^2 + \epsilon^2\right)}{2\sqrt{\gamma_0^2 + \epsilon^2}\left((a\delta g + \gamma_0)^2 + \epsilon^2\right)}, \tag{5.40}$$

while, since we are considering a closed system, the invariant heat reduces to the coherent heat. Therefore the heat takes the form

$$Q_c[\rho] = \frac{a^2\delta g^2\epsilon^2}{2\sqrt{\gamma_0^2 + \epsilon^2}\left((a\delta g + \gamma_0)^2 + \epsilon^2\right)}, \tag{5.41}$$

Their derivative with respect to g_0 are given by

$$\frac{dW_{inv}[\rho]}{dg_0} = -\frac{a^2\delta g\epsilon^2\left(a^4\delta g^4 + 3a^3\delta g^3\gamma_0 + 2a^2\delta g^2\gamma_0^2 + a\delta g\gamma_0\left(\gamma_0^2 + \epsilon^2\right) + \left(\gamma_0^2 + \epsilon^2\right)^2\right)}{2\left(\gamma_0^2 + \epsilon^2\right)^{3/2}\left((a\delta g + \gamma_0)^2 + \epsilon^2\right)^2} \tag{5.42}$$

$$\frac{dQ_c[\rho]}{dg_0} = -\frac{a^2\delta g^2\epsilon^2\left(\epsilon^2(2a\delta g + 3\gamma_0) + \gamma_0(a\delta g + \gamma_0)(a\delta g + 3\gamma_0)\right)}{2\left(\gamma_0^2 + \epsilon^2\right)^{3/2}\left((a\delta g + \gamma_0)^2 + \epsilon^2\right)^2}. \tag{5.43}$$

Furthermore, diagonal entropy can be computed using ρ_{11}^E and ρ_{22}^E.

Figure 5.5 reveals the behaviour of the work [panel 5.5(a)], heat [panel 5.5(b)], and entropy in the inset of [panel 5.5(b)] for distinct quenches from g_0 to $g = g_0 + \delta g$.

In particular, panel 5.5 (a) shows that the invariant work exhibits a similar behaviour to that observed for the derivative of the ground state energy of the model, as shown in Fig. 5.4. This

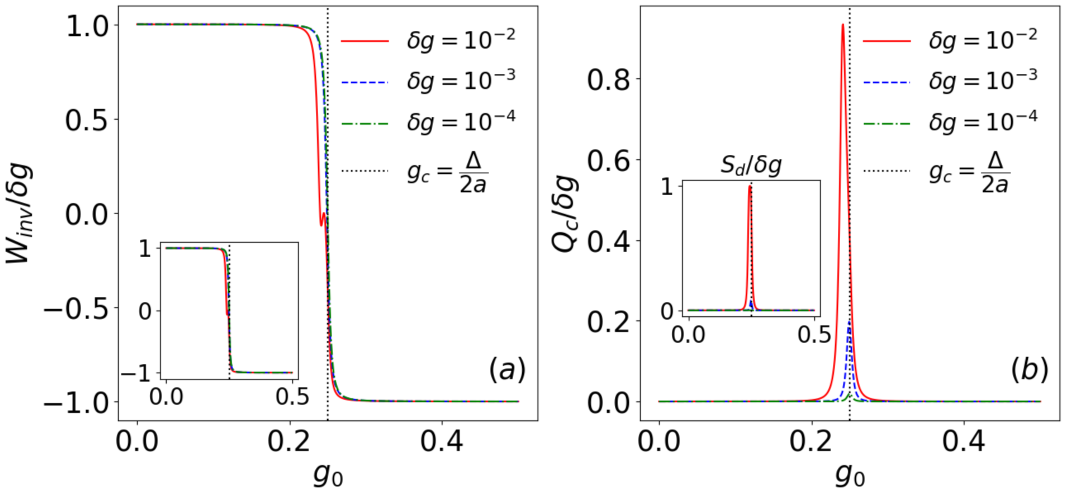

FIGURE 5.5: Invariant work (a), heat (b) and diagonal entropy per quench for Landau-Zener model. In the inset of coherent heat, we plot the diagonal entropy per quench. We set $a = 2$, $\Delta = 1$ and $\epsilon = 0.001$ for different values of the quench amplitude δg. The dotted vertical lines marks the critical point of the model.

similarity is especially pronounced in the regime of small quenches, i.e., $\delta g \to 0$. Furthermore, for small quenches, panel 5.5(b) indicates that the coherent heat approaches zero, suggesting a negligible contribution of energy associated with the change of basis during the quench. Indeed, for $Q_c[\rho] \approx 0$ and considering the system with no degeneracies, we can connect $W_{inv}[\rho]$ with the variation of the ground state energy with respect to the parameter g_0 as

$$\frac{dE_0}{dg_0} \approx \frac{2}{g_0} W_{\mathrm{inv}}[\rho], \tag{5.44}$$

which follows from the Hellman-Feynman Theorem[3] [122]. In fact, from this theorem we have

$$\frac{dE_0(g)}{dg} = \mathrm{Tr}\,\{\rho H_1\} = \frac{2}{g} W_{inv}[\rho] + \frac{2}{g} Q_c[\rho] \tag{5.45}$$

since $g \neq 0$, $H_1 = (1/g)(H(\tau) - H_0)$ and $\rho = \rho_{diag} + \rho_c$. This result is valid if and only if the spectrum of the Hamiltonian is not degenerated. In the particular case where $Q_c[\rho] \approx 0$, Eq. (5.45) have only contributions from the invariant work. Which justifies the correspondence between

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[3] **Hellman-Feynman Theorem**. Let H_λ be a Hamiltonian depending smoothly on a parameter λ, with normalized eigenstates $|\psi_\lambda\rangle$ and eigenvalues E_λ:

$$H_\lambda |\psi_\lambda\rangle = E_\lambda |\psi_\lambda\rangle$$

Then the derivative of the energy expectation value equals the expectation value of the Hamiltonian derivative:

$$\frac{dE_\lambda}{d\lambda} = \langle\psi_\lambda|\frac{\partial H_\lambda}{\partial \lambda}|\psi_\lambda\rangle = \mathrm{Tr}\left\{\frac{\partial H_\lambda}{\partial \lambda}\rho_\lambda\right\}$$

where $\rho_\lambda = |\psi_\lambda\rangle\langle\psi_\lambda|$.

the variation of the ground state energy and the invariant work in Fig. 5.4 and Fig. 5.5 (a).

Another interesting aspect to consider in the Landau-Zener model is the case with energy level crossing, i.e., $\epsilon = 0$. In this case, the contribution of heat is zero, which is expected since $[H_0, H_\tau] = 0$. However, the model exhibits degeneracy at the critical point $g_0 = \Delta/4a$. At this point, the thermodynamic group $\mathcal{G}_\mathrm{T}$ is isomorphic to the group $\mathcal{U}(2)$. Consequently, the Haar measure induced by the thermodynamic group is $\mathrm{d}\,\mathcal{G}_\mathrm{T}^{g_c} = \mathrm{d}\,\mu\,[\mathcal{U}(2)]$. Therefore, it follows that the expression for the invariant work is modified to $W_\mathrm{inv}[\rho] = -a\delta g/2\,\mathrm{sgn}\,(g_0 - \Delta/2)$, where $\mathrm{sgn}(\cdot)$ denotes the sign function.

Signatures of the QPT can be seen in the derivatives of invariant work and heat. As the system approaches the critical point of the phase transition, these quantities exhibit divergent behaviour. This divergence is visually evident in Fig. 5.6.

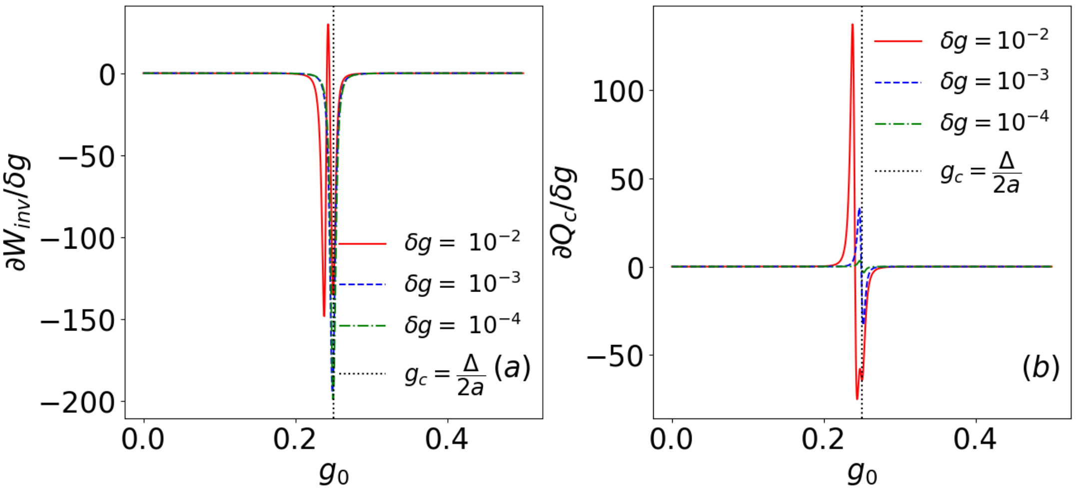

FIGURE 5.6: Derivative of invariant work (a) and heat (b) for different quenches for the Landau-Zener model. In these plots, we set $a = 2$, $\Delta = 1$, and $\epsilon = 0.001$. The divergence appearing in the invariant work (coherent heat) for small (large) values of the quench amplitude is evident.

Note that the results obtained here are consistent with the expected physical understanding of the Landau-Zener model and its quantum phase transition. In particular, the coherent heat becomes significantly relevant near the system's critical phase transition point, which is associated with the loss of control over non-adiabatic transitions and the generation of quantum coherence in the energy basis around the model's phase transition. On the other hand, the contribution of coherent heat is negligible in regions far from the critical point. This behavior arises because we are dealing with a physical system subjected to small quenches and confined to a low-dimensional Hilbert space. In this context, as demonstrated by the Hellmann-Feynman theorem, our analysis aligns with previous findings in the literature [92] regarding the model's phase transition, particularly the identification of the invariant work as the system's order parameter.

5.4 QPT in Lipkin-Meshkov-Glick model

In Chapter 4, we briefly presented a particular case of the Lipkin-Meshkov-Glick model [99–101]. Now, we will return to discuss this model, focusing on its quantum phase transition. In this sense, let us consider the Hamiltonian:

$$H_g = -\frac{k}{2j}\left(J_z^2 + \gamma J_y^2\right) - gJ_x. \tag{5.46}$$

The parameter $0 \leq \gamma \leq 1$ denotes an anisotropy constant of the model, while the other constants are described as in Chapter 4, that is, $J_\alpha = \sum_{i=1}^{N} \sigma_i^\alpha/2$; $(\alpha = x, y, z)$ are the collective spin operators, with σ_i^α denoting the α Pauli matrix acting on the i-th site of a chain of $N = 2j$ sites, where j is the total angular momentum and $k > 0$ denotes the coupling between the spins. The parameter $g \geq 0$ is the strength of the magnetic field along the x-axis.

As mentioned in Chapter 4, the LMG model has a variety of interesting applications. Furthermore, the model exhibits a wealth of extremely interesting physical phenomena, such as the presence of chaos [123] and critical phenomena like quantum phase transitions (QPT) [124, 125], excited state phase transitions (ESQPT) [126, 127], and dynamic phase transitions (DQPT) [128, 129].

The quantum phase transition in the LMG model occurs in the thermodynamic limit as $j \to \infty$. In this scenario, the parity symmetry is broken as the magnetic field transitions from $g < g_c$ (ferromagnetic phase) to $g > g_c$ (paramagnetic phase), with $g_c = k$ being the critical point of the equilibrium phase transition [124]. A specific characteristic of these two phases is related to the degeneracies of the Hamiltonian. While the ferromagnetic phase is doubly degenerate, the paramagnetic phase is non-degenerate. Figure 5.7 illustrates these configurations.

The quantum phase transition in the LMG model can be identified through some quantities that serve as order parameters for the model [92, 125]. In fact, two order parameters that we can highlight are the average magnetizations of the spin chain and the transverse field, which are given respectively by:

$$\langle J_x \rangle = \mathrm{Tr}\{\rho_g^{gs} J_x\} \text{ and } \langle J_z \rangle = \mathrm{Tr}\{\rho_g^{gs} J_z\} \tag{5.47}$$

where ρ_g^{gs} denotes the density operator associated with the ground state of the Hamiltonian H_g in Eq. (5.46) for each value of g of the external magnetic field. In Figure 5.8, we present the behavior of these order parameters for the QPT in the LMG model.

Having made this brief discussion, we will now evaluate how the formalism of the thermodynamic group $\mathcal{G}_\mathrm{T}$ connects with the QPT in the LMG model.

Indeed, the presence of degeneracies in one of the phases of the LMG model leads to a modification of the structure of the thermodynamic group. Thus, unlike the Landau-Zener model, here

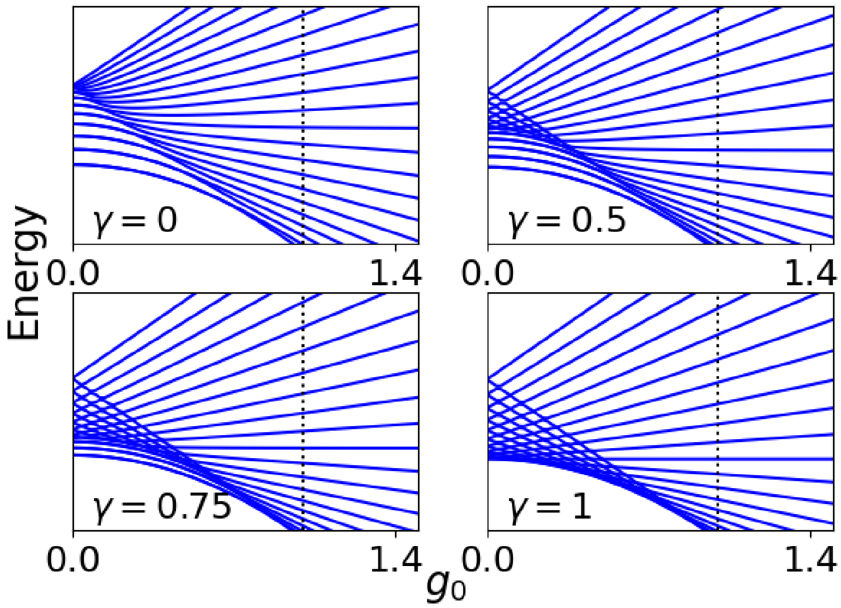

FIGURE 5.7: Energy spectrum of LMG model in Eq. (5.46) for different values of γ. Here we used $j = 10$ for all panels. The vertical dotted line marks the critical point of the model.

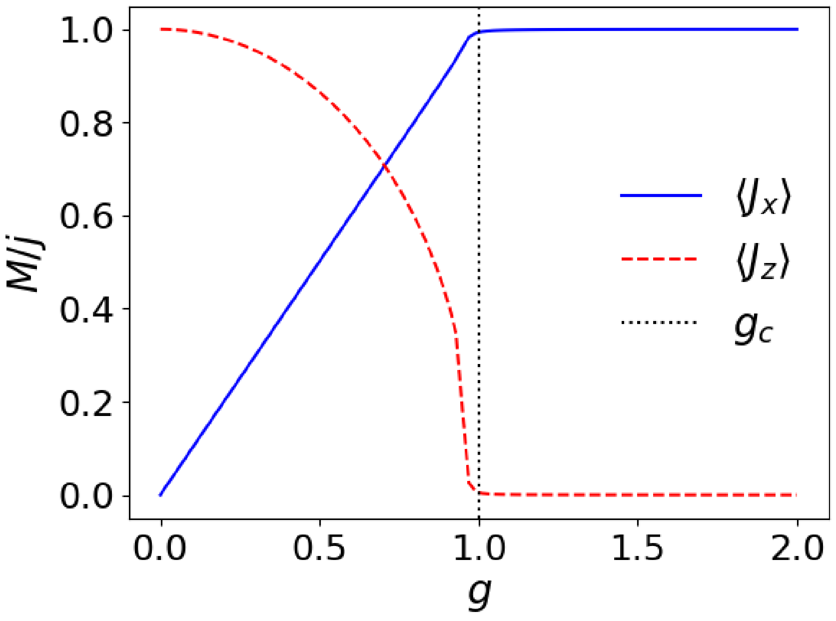

FIGURE 5.8: Average magnetizations of the spin chain $\langle J_z \rangle$ and the transverse magnetic field $\langle J_x \rangle$ normalized by j in the LMG Hamiltonian in Eq. (5.46) as order parameters.

the thermodynamic group has the general form given by:

$$\mathcal{G}_{\mathrm{T}} = \mathcal{U}(2) \times \mathcal{U}(2) \times \mathcal{U}(2) \times \ldots \times \mathcal{U}(2) \tag{5.48}$$

for the ferromagnetic phase, since in the thermodynamic limit, the energy levels are all doubly degenerate. On the other hand, in the paramagnetic phase, the thermodynamic group reduces to the following structure:

$$\mathcal{G}_{\mathrm{T}} = \mathcal{U}(1) \times \mathcal{U}(1) \times \mathcal{U}(1) \times \ldots \times \mathcal{U}(1). \tag{5.49}$$

From the perspective of the thermodynamic group, the ferromagnetic phase has greater redundancy associated with the topological structure of the $\mathcal{G}_{\mathrm{T}}$-group compared to the paramagnetic phase.

Moreover, note that since we cannot practically reach the thermodynamic limit for a spin chain associated with the LMG model, we are essentially describing a finite-dimensional system. In this case, the structure of degeneracies in the model is subtly different; in fact, for values of $g < g_c$, there exists a certain number of eigenenergies that are doubly degenerate. However, in finite dimensions, as the intensity of the magnetic field g is increased, the degeneracies that initially exist solely due to the coupling of the spins are broken.

As a result, as the degeneracies of the model are broken and the energy levels are split, the thermodynamic group exhibits a symmetry breaking in one of its structures. Nonetheless, note that the density operator ρ_{dd}^{E} will not reduce to a complete dephasing as occurs in the Landau-Zener model that we explored in the previous section. In this context, we must evaluate, for each value of g associated with the Hamiltonian H_g, the structure of the thermodynamic group in order to assess the Haar average of the density operator.

Now, we will proceed to obtain the expressions associated with invariant work and heat. To this end, we consider the time-dependent counterpart associated with the Hamiltonian in Eq. (5.46) as

$$H_g(t) = -\frac{k}{2j}\left(J_x^2 + \gamma J_y^2\right) - (g_0 + \delta g \theta(t-\tau))J_z. \tag{5.50}$$

We then have $H_{g_0} = -(k/2j)\left(J_z^2 + \gamma J_y^2\right) - g_0 J_x$ and $H_1 = -J_x$. In the present case, it is not possible to obtain analytical expressions for the eigenvectors and/or eigenvalues in terms of the control parameter g as we did for the Landau-Zener model. Therefore, we investigate this model using numerical methods. However, before proceeding, we will rewrite the expressions for the invariant work and heat in the more convenient form:

$$W_{inv}[\rho] = -\frac{\delta g}{2}\operatorname{Tr}\left\{\rho_{dd}^{E} J_x\right\} \text{ and } Q_c[\rho] = -\frac{\delta g}{2}\operatorname{Tr}\left\{\left(\rho^{E} - \rho_{dd}^{E}\right) J_x\right\} \tag{5.51}$$

this expressions follows from Eq. (5.26) e Eq. (5.28) respectively.

Here, we proceed by fixing the quench amplitude at $\delta g = 0.01$ and the anisotropy constant at $\gamma = 0.75$. Previous numerical analyses have shown that the qualitative behavior of the quantities is independent of these choices.

A direct consequence of the theory emerges from the expression for the invariant work. It is an order parameter for the system, since the magnetisation $\langle J_\alpha \rangle = \mathrm{Tr}\{\rho J_\alpha\}$ (with $\alpha = x, y, z$) is the usual order parameter in Eq. (5.47) signalling the quantum phase transition in the this case [92]. Por outro lado, o calor coerente aqui é dado pela diferença entre as magnetizações, na direção x, associadas aos estados ρ (que é o parâmtro de ordem usual do sistema) e o próprio trabalho invariante, isto é:

$$\begin{aligned} Q_c[\rho] &= -\frac{\delta g}{2}\,\mathrm{Tr}\left\{\rho^E J_x\right\} - \left(-\frac{\delta g}{2}\,\mathrm{Tr}\left\{\rho^E_{dd} J_x\right\}\right) = -\frac{\delta g}{2}\left(\langle J_x \rangle_{\rho^E} - \langle J_x \rangle_{\rho^E_{dd}}\right) \\ &= -\frac{\delta g}{2}\,\langle J_x \rangle_{\rho^E} - W_{inv}[\rho], \end{aligned}$$

ou seja, o calor coerente e trabalho invariante ficam conectados com o parâmetro de ordem do modelo. Na Fig. 5.9 os resultados numéricos associados ao trabalho invariante e suas derivadas.

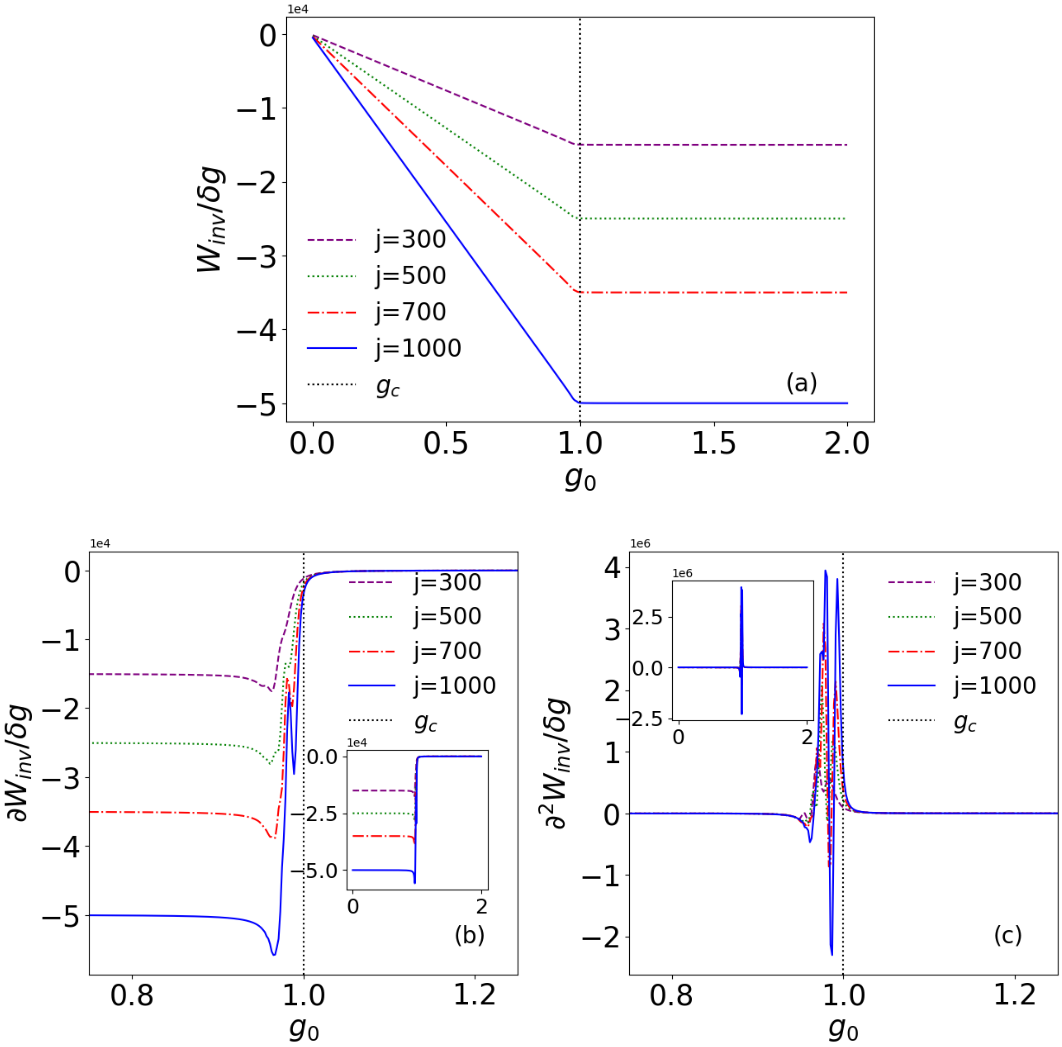

FIGURE 5.9: Thermodynamics of the LMG model. Panel (a) shows the invariant work, normalized by the quench, considering distinct values of j. Next, we see in Panel (b) the first derivative of the invariant work with respect g_0, normalized by quench amplitude. Panel (c) revels the divergence of second derivative of the invariant work in vicinity of the quantum critical point.

As expected, the qualitative profile of the invariant work reveals its similarity with the behavior of the model's order parameter for the quantum phase transition (QPT). Moreover, the signature of an apparent divergence emerges only in the second derivative of the work, consistent with the fact that we are dealing with a first-order phase transition.

Another key observation concerns the behavior of the invariant work, which remains constant for $g_0 > 1$. That is, quenches performed in the paramagnetic phase do not modify the work. This interesting result can be explained by the fact that for $g_0 > 1$, the system is in a strong-coupling regime between the spin chain and the transverse magnetic field. Consequently, infinitesimal quenches cannot generate significant work in this regime.

Regarding the coherent heat, its behavior is shown in Fig. 5.10. We observe that the heat undergoes an abrupt change near the model's critical point, while the divergence of its derivative with respect to the quench clearly marks this transition.

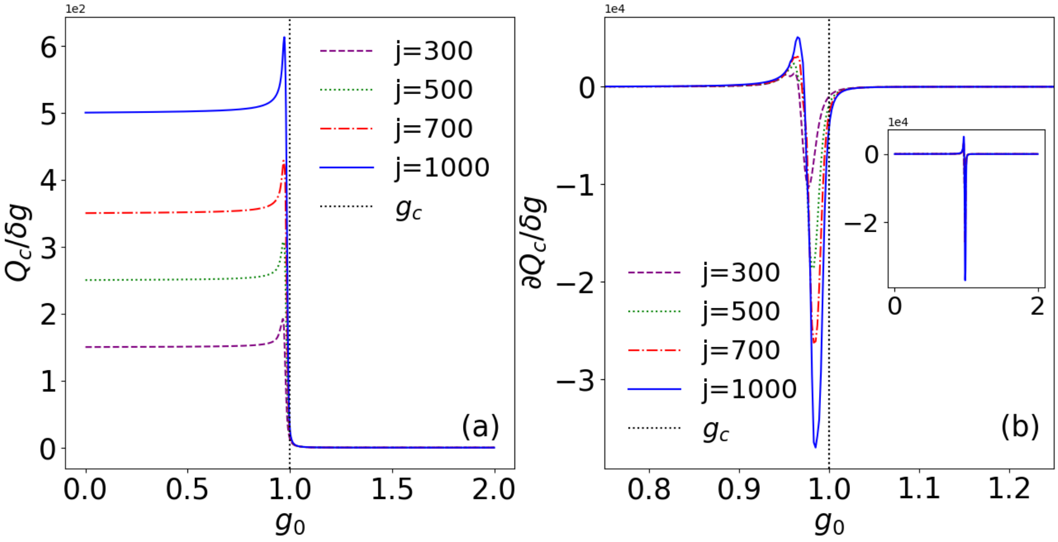

FIGURE 5.10: Invariant heat in Panel (a) and its derivative in Panel (b), for the LMG model considering different values of j per quench.

Several noteworthy features emerge from the behavior of these invariant quantities. Indeed, we again observe a peak in the coherent heat at the model's critical point, which—as in the Landau-Zener model—is linked to the loss of physical information due to the phase transition, generating quantum coherences in the energy eigenbasis. However, in the paramagnetic phase, the heat vanishes asymptotically, a consequence of the strong-coupling regime between spins and the transverse field. Crucially, as the coherent heat disappears, the invariant work in this phase converges arbitrarily close to the model's true order parameter.

We now discuss the thermodynamic entropy $S_{\mathcal{G}_T}$ for this system, which—unlike in the Landau-Zener model—does not coincide with the diagonal entropy due to the presence of degeneracies. As previously mentioned, the ferromagnetic phase ($g < g_c$) is doubly degenerate, whereas the paramagnetic phase ($g > g_c$) is entirely non-degenerate. Thus, we expect markedly distinct behaviors of $S_{\mathcal{G}_\mathrm{T}}$ in the two phases, as illustrated in Fig. 5.11.

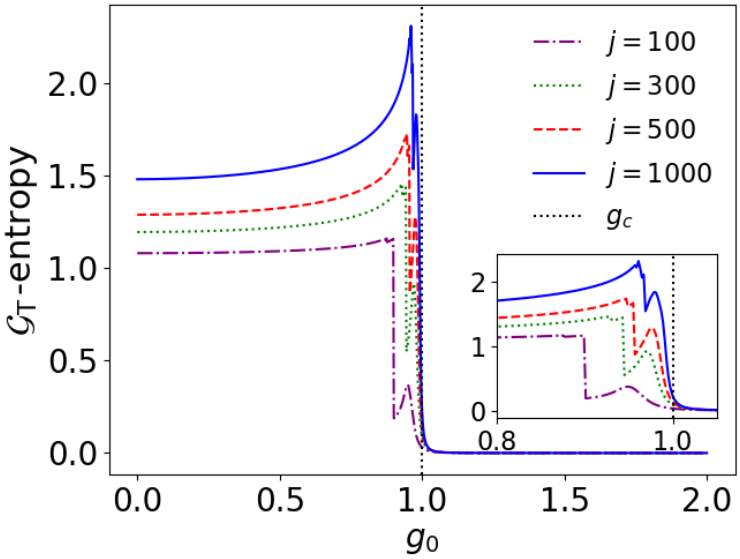

FIGURE 5.11: Thermodynamic $\mathcal{G}_\mathrm{T}$-entropy for the ground state of the LMG model as a function of g_0, considering different values of j. The inset shows a zoom near the critical point, highlighting the abrupt change in $S_{\mathcal{G}_\mathrm{T}}$ at criticality.

A striking similarity exists between the $\mathcal{G}_\mathrm{T}$-entropy in Fig. 5.11 and the heat displayed in Fig. 5.10(a). This is no coincidence but rather a direct consequence of the underlying theory, which ties both quantities to the production of quantum coherence in the energy eigenbasis and the degeneracies present in the ferromagnetic phase. In particular, as discussed in Chapter 4, this result stems from the fact that both the gauge entropy and the coherent heat arise from the non-unitary term in the effective coarse-grained state dynamics. This finding further corroborates and extends the interpretation of heat proposed in Ref. [3].

Moreover, Fig. 5.11 clearly shows a tendency for an abrupt change in $S_{\mathcal{G}_\mathrm{T}}$ in the vicinity of the critical point. Such change occurs precisely at the point where the degeneracies of the system are completely extinguished due to the competition between the contributions of the spin coupling and the external magnetic field. The extinction of degeneracies before the critical point occurs because we are dealing with a finite-dimensional system.

However, as shown in the Fig. 5.11, this point tends to shift to the critical point of the model for larger dimensions, where we approach the thermodynamic limit. Additionally, we observe that the abrupt change in $S_{\mathcal{G}_\mathrm{T}}$ is more pronounced in chains with fewer spins, which is associated with the contributions of degeneracies being more significant in systems further away from the thermodynamic limit.

Accordingly, we analyze $S_{\mathcal{G}_\mathrm{T}}$ in comparison with the diagonal entropy S_d, highlighting the contributions of degeneracies as quantified by the Holevo asymmetry measure S_Γ and also the effect of the size of the chain. First, we observe from Fig. 5.12 that oscillatory behavior of the Holevo asymmetry measure in the vicinity of the critical point arises from the breaking of energy level degeneracies, which results in modifications to the structure of the thermodynamic group $\mathcal{G}_{\mathrm{T}}$. As the value of j increases, the oscillations in the Holevo asymmetry S_{Γ} decrease near the critical point and eventually vanish at the quantum phase transition.

Then, from the point of view of the Holevo asymmetry measure, degeneracies produce asymmetry and consequently increase the randomness and entropy of the state. However, it is the relationship between the total volume of the subspaces $\mathcal{H}_k$ and the changes in degeneracies that leads to abrupt modifications in the thermodynamic entropy. Consequently, we expect a greater impact of degeneracies in lower-dimensional systems, since the Haar averages contained in S_{Γ} are significant with respect to the contributions of populations coming from the diagonal entropy.

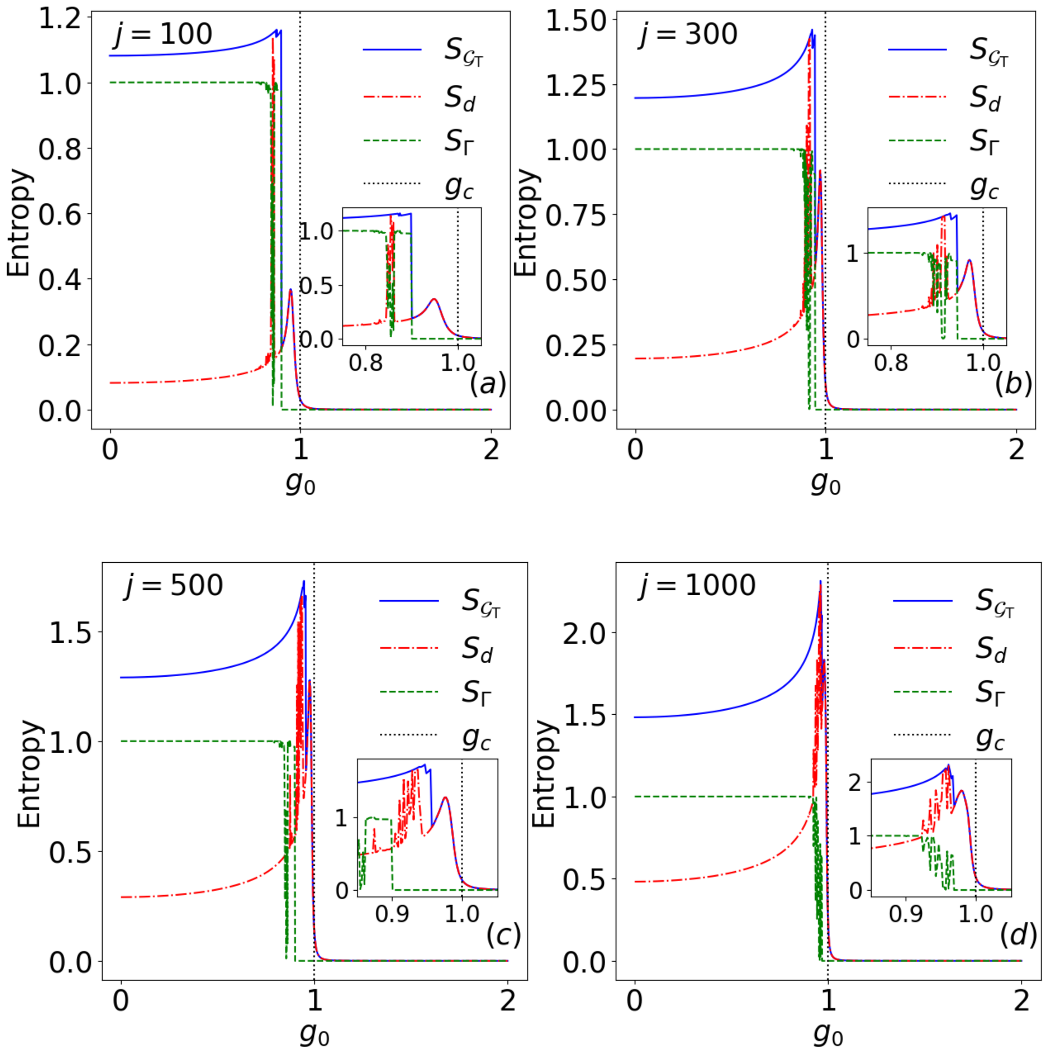

FIGURE 5.12: Comparative of thermodynamic gauge entropy $S_{\mathcal{G}_{\mathrm{T}}}$, diagonal entropy S_d and Holevo asymmetry measure S_{Γ} for $j = 100, 300, 500, 1000$ in Panels (a), (b), (c) and (d) respectively. The insets in all panels correspond to a zoom in the vicinity of the critical point.

However, this scenario is modified as we consider systems with larger dimensions, as already indicated in Fig. 5.12 (c). In this regard, in Fig. 5.13 we study how the entropies behave in the vicinity of the critical point when we consider higher dimensional models. Thus, for large values of j, near the critical point of the phase transition, the diagonal entropy approaches $S_{\mathcal{G}_\mathrm{T}}$, while the Holevo asymmetry fluctuates around values close to zero. Indeed, this behaviour emerges because the contributions of the remaining degeneracies are not as significant as in smaller dimensions, as shown by the S_Γ curve in Figs. 5.12 and 5.13. Therefore, from Eq. (4.64) it follows that near the critical point $|S_{\mathcal{G}_\mathrm{T}} - S_d| = S_\Gamma$ and, since S_Γ becomes increasingly less significant, we conclude that the $\mathcal{G}_\mathrm{T}$-entropy and the diagonal entropy approach each other. Thus, the Holevo asymmetry acts as a parameter that determines the continuity of the thermodynamic gauge entropy.

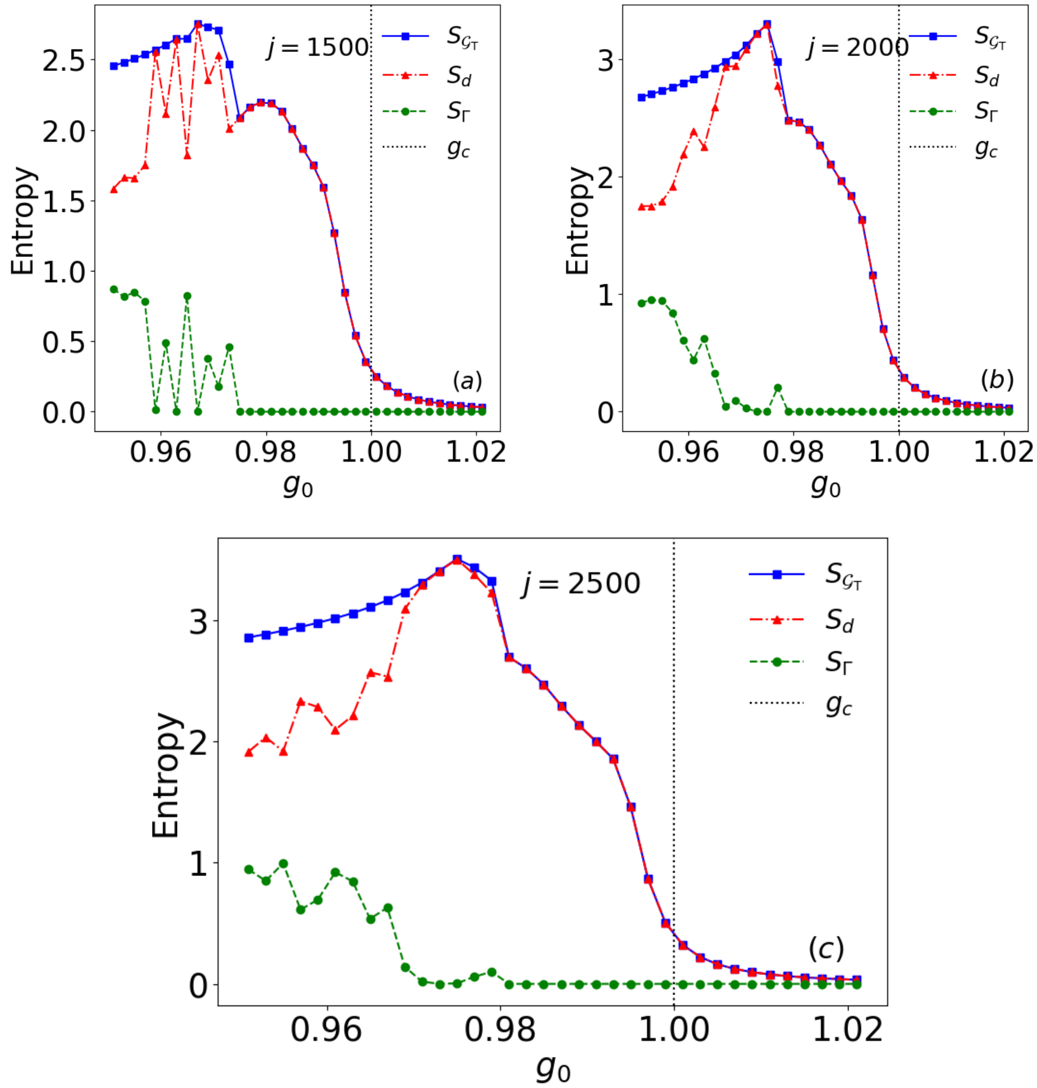

FIGURE 5.13: Comparative of Thermodynamic gauge entropy $S_{\mathcal{G}_\mathrm{T}}$, diagonal entropy S_d and Holevo assymetry measure S_Γ in the vinicity of the quantum critical point in the LMG model for $j = 1500, 2000, 2500$ in Panels (a), (b) and (c) respectively.

On the other hand, for quenches occurring after the critical point of the phase transition, we observe that $S_{\mathcal{G}_\mathrm{T}}$ asymptotically tends to zero. Indeed, after the critical point, the thermodynamic group is always given by $\mathcal{G}_{\mathrm{T}} = \prod_{k=1}^{d} \mathcal{U}(1)$, and consequently, the diagonal part of the states ρ in the energy basis becomes increasingly symmetric with respect to the group $\mathcal{G}_{\mathrm{T}}$, thereby asymptotically reducing the entropy.

Chapter 6

Discussion and Future perspective

In this study, we develop a quantum thermodynamics theory structured as a gauge theory for the thermodynamic group, following the approach outlined in [3] while considering limited information access to the system. This methodology leverages the principle of gauge invariance, inspired by conventional gauge theories in modern physics, and is founded on the premise that only certain system observables are measurable. Consequently, thermodynamic quantities emerge as Haar averages associated with this gauge group. As a result, we establish invariant formulations for heat, work, and entropy applicable to general quantum systems, thereby providing a comprehensive quantum thermodynamics framework rooted in gauge invariance. To demonstrate the physical implications of this framework, we apply the theory to quantum critical systems.

A significant achievement of this theory is the unambiguous separation of a system's energy into heat and work components, addressing a long-standing controversy in quantum thermodynamics, particularly for closed quantum systems. Specifically, we show that the hypothesis of limited information access redistributes the energy into: (i) a new work quantity (invariant work), associated purely with population elements, and (ii) a new heat quantity (coherent heat) connected to density matrix coherences.

Furthermore, we provide a clear physical interpretation of these quantities by demonstrating their equivalence to Alicki's standard quantum thermodynamics formulation [15] for the effective density operator obtained through coarse-graining over all transformations comprising the thermodynamic group. The dynamics of this group is governed by a non-unitary equation where the non-unitary term precisely generates the coherent heat contribution. Thus, we establish that coherent heat represents energy inaccessible to the system, emerging from lack of control and fundamentally linked to quantum effects - particularly modifications in quantum coherences and non-adiabatic transitions in the energy basis. Conversely, the invariant work naturally corresponds to the system's effective work after this energy loss to coherent heat, depending solely on population contributions, thereby aligning with classical thermodynamics' notion of work.

Another fundamental result is our definition of thermodynamic entropy. By interpreting von Neumann entropy as a quantum information measure, we derive a unified thermodynamic entropy that remains invariant under the thermodynamic group. This entropy decomposes into two components: the well-known diagonal entropy [22] and a purely quantum contribution arising from system degeneracies. The gauge-invariant entropy derived within our framework satisfies all key requirements for thermodynamic entropy. Notably, in the classical limit, the quantum contribution vanishes, reducing the gauge-invariant entropy to diagonal entropy - thus emerging naturally for non-degenerate or classical Hamiltonians in our formalism.

Moreover, thermodynamic entropy is fundamentally connected to the development of quantum coherences in the energy eigenbasis, which naturally correlates with invariant and coherent heat. Through the dynamical equation for the coarse-grained state, we demonstrate that gauge entropy variation is generated by the same operator responsible for coherent heat, thereby explaining the qualitative connection between these quantities that was numerically observed in Ref. [3] and is now rigorously established in this work. The physical basis for this connection lies in the well-documented relationship between heat and quantum coherences [28]. From a thermodynamic perspective, our ability to manipulate systems is inherently constrained - experimental measurements typically access few observables (often just energy). Consequently, quantum coherence generation increases uncertainties in these observables, producing entropy. Within our gauge framework (and in Ref. [3]), this connection emerges naturally.

These concepts become particularly evident when applying the theory to paradigmatic quantum critical systems like the Landau-Zener and Lipkin-Meshkov-Glick (LMG) models. The Landau-Zener model describes a non-degenerate two-level system, while the LMG Hamiltonian represents fully connected spin chains exhibiting doubly degenerate phases. In both cases, the invariant thermodynamic quantities developed herein show remarkable sensitivity to the quantum phase transitions in these models, clearly revealing the intrinsically quantum nature of thermodynamics.

6.1 Future perspective

Certainly, we have managed to develop and extend several results initially obtained by Céleri and Rudnicki in [3]. However, we recognize that the framework presented here is still a modest development compared to the various perspectives that can be pursued. Moreover, we can categorize these paths into two types: the first is associated with potential generalizations of the formalism, and the second is aimed at expanding the scope of applications to physical problems beyond critical systems. In this context, in the following two subsections, we will comment on each of these paths and discuss how each possibility we outline could be developed.

6.1.1 Potential for Generalizations of the Theory

Firstly, we will highlight some aspects related to generalizing the theory. Certainly, the reader might imagine that an initial approach for this generalization would be simply to relax the initial assumptions made in Section 3.2. However, assumptions (i) and (ii) do not have much potential for generalization since the conditions they impose are sufficiently reasonable.

However, assumptions (iii) and (iv) can indeed be relaxed and then extended to a more general framework, such that in a certain limit, the formalism developed in this work is recovered. Additionally, there are other extensions we consider regarding the geometric nature of the theory, due to our development being based on a non-abelian Lie group. Below, we discuss these potential generalizations of the theory in some detail.

I) (Generalized invariance principle). As an initial perspective, we bring up the discussion at the end of Chapter 3. Specifically, the development of the gauge invariance principle constructed around a different observable. In effect, the Definition 3.53 of generalized invariance alters the Haar measure, and consequently, the expressions obtained for heat and work in Chapters 4 and 5 will need modification. Regarding entropy, this generalization only affects the type of coarse-graining applied; in this sense, Gibbs states may no longer remain invariant, and therefore, the $\mathcal{G}$-entropy becomes inconsistent with Gibbs entropy for thermal states.

II) (Generalized invariant quantities). Another potential generalization is extending the Definition 3 of invariant quantities. This possibility arises from the work of Marvian and Spekkens [84], where the Haar average is defined in a non-uniform manner by introducing a weight function $\phi(\mathcal{G})$ associated with the thermodynamic gauge group. Consequently, these expressions would become:

$$F_{inv}[\rho(t)] \quad \rightarrow \quad F^{p}_{inv}[\rho(t)] = \int \mathrm{d}\mathcal{G}_{\mathrm{T}}\, \phi(\mathcal{G}) F_u[V_t\rho(t)V_t^{\dagger}] \tag{6.1}$$

$$\rho_{dd} \quad \rightarrow \quad \rho^{\phi}_{dd} = \int \mathrm{d}\mathcal{G}_{\mathrm{T}}\, \phi(\mathcal{G}) V_t\rho(t)V_t^{\dagger}. \tag{6.2}$$

However, modifying Definition 3 by introducing the weight ($\phi(\mathcal{G})$) is not a trivial matter, particularly concerning the physical interpretation of this function. It alters the Haar average in such a way that certain elements of the Haar group are "privileged" in this process. Questions like: Why should this average select certain elements? must be considered. Thus, the feasibility of this generalization requires a discussion on suitable classes of weight functions $\phi(\mathcal{G})$ that align with the thermodynamic context. A priori, choosing $\phi(\mathcal{G})$=1 , corresponding to the uniform Haar average case, seems to be the most appropriate choice.

III) (Geometric/topological description of the theory). The thermodynamic gauge group (3.28) is a Lie group composed of the product of several unitary groups $\mathcal{U}(n_t^k)$. Consequently, $\mathcal{G}$ is a differentiable manifold, and thus, the gauge group inherently possesses a geometric and topological nature. In this context, a potential pathway for future developments would be the formalization of the theory from a geometric and topological perspective, similar to how conventional gauge theories are constructed. This would involve defining and constructing elements such as bundles and connections. Naturally, a critical question would be whether a Lagrangian functional exists within the theory.

6.1.2 Scope for applications of the theory

In addition to the development of the theoretical formalism, we also highlight several potential applications to physical problems.

I) Since the numerical results obtained in Chapter 4 and Chapter 5 show a close qualitative relationship between coherent heat and $\mathcal{G}_{\mathrm{T}}$-entropy, the possibility arises of analytically deriving an expression that directly relates coherent heat and the entropy of the theory. In particular, a possible Clausius-like relation from classical thermodynamics could be considered as a starting point for a new generalized relation within our theory.

II) While we have demonstrated the relationship between thermodynamic quantities and criticality effects associated with quantum phase transitions (QPT), it is natural to question whether critical effects could also emerge in systems exhibiting dynamical criticality [130].

III) Moreover, we observe that the structure of the thermodynamic group, particularly how the group is modified as certain parameters of the Hamiltonian are altered, could suggest a framework for identifying excited state quantum phase transitions (ESQPT).

IV) Finally, we have thus far discussed applications in the context of closed systems. However, considering open systems is another avenue to explore, particularly in evaluating how the notions of invariant heat and work might alter the determination of thermal machine efficiency.

Appendix A

Some technical results

A.1 Mathematical results

Definition 8. *(σ-algebra [131]) A collection $\mathcal{A}$ of subsets of Ω, meaning $\mathcal{A} \subset P(\Omega)$, where $P(\Omega)$ denotes the power set of Ω, is said to be a σ-algebra on Ω if the following requirements are satisfied:*

(i) $\emptyset \in \mathcal{A}$ *and* $\Omega \in \mathcal{A}$.

(ii) If $A \in \mathcal{A}$, *then* $A^c \equiv \Omega \backslash A \in \mathcal{A}$.

(iii) If $\{A_n, n \in \mathbb{N}\}$ *is an arbitrary countable collection of elements of* $\mathcal{A}$, *then* $\bigcup_{n \in \mathbb{N}} A_n$ *is also an element of* $\mathcal{A}$.

Definition 9. *(Measure [131]) Let Ω be a non-empty set and $\mathcal{A}$ a σ-algebra on Ω (for the definition, see Chapter 28, page 1483). We will present the formal concept of a measure. A measure on $\mathcal{A}$ is a function μ that assigns to each element of the σ-algebra $\mathcal{A}$ a real number ≥ 0 or infinity, that is, $\mu : \mathcal{A} \to \mathbb{R}_+ \cup \{\infty\}$, such that the following conditions are satisfied:*

(i) $\mu(\emptyset) = 0$.

(ii) If $A_i, i \in \mathbb{N}$, *is a countable and disjoint collection of elements of* $\mathcal{A}$, *then*

$$\mu\left(\bigcup_{n \in \mathbb{N}} A_n\right) = \sum_{n \in \mathbb{N}} \mu\left(A_n\right) \tag{A.1}$$

The second property is sometimes referred to as countable additivity, or σ-additivity.

Definition 10. *(Measure Spaces). Let Ω be a non-empty set, $\mathcal{A}$ a σ-algebra on $P(\Omega)$ (the power set of Ω), and μ a measure on $\mathcal{A}$ then:*

I) The pair (Ω, μ) *is called a measurable space.*

I) The triple $(\Omega, \mathcal{A}, \mu)$ *is called a measure space.*

II) If in a measure space we have $\mu(\Omega) = 1$, *then the triple* $(\Omega, \mathcal{A}, \mu)$ *is called a probability space.*

Theorem 7. *Let* $(\Omega, \mathcal{A}, \mu)$ *and* $(\Omega', \mathcal{A}', \gamma)$ *two measure spaces* σ*-finite and* $v = \mu \times \gamma$.

a) (Tonelli Theorem). if $f : \Omega \times \Omega' \to \overline{\mathbb{R}}$ *is a function* $\mathcal{A} \times \mathcal{A}'$*-mensurable and non-negative, then the functions:*

$$\omega \to \int_{\Omega'} f(\omega, \cdot) d\gamma \quad e \quad \omega' \to \int_{\Omega} f(\rho, \omega') \, d\mu$$

are $\mathcal{A}$ *e* $\mathcal{A}'$ *mensurable respectively and*

$$\int_{\Omega} \left[\int_{\Omega'} f(\omega, \cdot) d\gamma \right] d\mu = \int_{\Omega'} \left[\int_{\Omega} f(\cdot, \omega') \, d\mu \right] d\gamma = \int_{\Omega \times \Omega'} f dv$$

b) (Fubini). if f *is* μ*-integrable, then* $f(\omega, \cdot)$ *é* γ*-integrable for for almost everything* $\omega[\mu]$, *e* $f(\cdot, \omega')$ *is* μ*-integrable for almost everything* $\omega'[\gamma]$

$$\int_{\Omega} \left[\int_{\Omega'} f(\omega, \cdot) d\gamma \right] d\mu = \int_{\Omega'} \left[\int_{\Omega} f(\circ, \omega') \, d\mu \right] d\gamma = \int_{\Omega \times \Omega'} f dv.$$

Proof. See Ref. [132] Theorem 5.2.2. □

More details on measure and integration theory, particularly regarding the Lebesgue measure, Hausdorff measure, and other measures, can be found in Refs. [131–133].

A.2 Quantum information theory

Quantum information theory is, without a doubt, the foundation for the developments presented in this work. Indeed, throughout the text, we continuously use methods, definitions, and results from this theory to construct the thermodynamics of the group $\mathcal{G}_{\mathrm{T}}$. With this in mind, in this appendix, we will present some of these definitions and results, which, in general, we will also seek to demonstrate, aiming for this appendix to serve not only as a complement to the main text but also as an educational resource for certain readers. In this sense, we will begin with the definition of a quantum channel, which is one of the fundamental elements in our work.

Definition 11. *(Quantum channel [41]) Let* $\mathcal{L}(\mathcal{H}^{d_1})$ *and* $\mathcal{L}(\tilde{\mathcal{H}}^{d_2})$ *be two spaces of density operators associated with the Hilbert spaces* $\mathcal{H}^{d_1}$ *and* $\tilde{\mathcal{H}}^{d_2}$, *respectively. We define a quantum channel (or quantum operation) as the map*

$$\begin{aligned} \mathcal{E} : \mathcal{L}(\mathcal{H}^{d_1}) &\to \mathcal{L}(\tilde{\mathcal{H}}^{d_2}) && \text{(A.2)} \\ \rho \in \mathcal{L}(\mathcal{H}^{d_1}) &\to \tilde{\rho} = \mathcal{E}(\rho), && \text{(A.3)} \end{aligned}$$

which satisfies the following properties:

A1. First, $\mathrm{tr}[\mathcal{E}(\rho)]$ *is the probability that the process represented by* $\mathcal{E}$ *occurs when* ρ *is the initial state. Thus,* $0 \leq \mathrm{tr}[\mathcal{E}(\rho)] \leq 1$ *for any state* ρ*.*

A2. Second, $\mathcal{E}$ *is a convex-linear map on the set of density matrices, that is, for probabilities* $\{p_i\}$*,*

$$\mathcal{E}\left(\sum_i p_i \rho_i\right) = \sum_i p_i \mathcal{E}\left(\rho_i\right).$$

A3. Third, $\mathcal{E}$ *is a completely positive map.*

This definition above reflects the choice to treat a quantum channel in an axiomatic manner. Indeed, this definition does not, a priori, assign a possible physical meaning to this map. However, the choice of the properties above can be understood as being motivated by an objective physical meaning. In fact, property $A1$ arises from the intrinsic probabilistic nature of quantum mechanics; in particular, if the inequality above is saturated, i.e., $\mathrm{tr}[\mathcal{E}(\rho)] = 1$, then we say that the quantum channel is a trace-preserving operation. Moreover, property $A2$ arises from the requirement that the quantum channel be linear, and thus convexity is achieved. Finally, property $A3$ ensures that the description of the evolution of a quantum state by the map is completely positive, consequently guaranteeing a valid physical reality.

Indeed, one of the basic applications of quantum channels is associated with the description of the evolution of a state ρ to a final state $\tilde{\rho}$. In closed systems, this evolution is governed by the Schrödinger equation, which is then described by a unitary operator U. However, for open quantum systems, there is no closed description in a single equation. Nevertheless, by considering the system of interest plus the environment interacting with it, we can treat the complete system (system + environment) as a closed system whose evolution is guided by a unitary operator. Below, in Figure A.1, we schematically illustrate these two evolutions based on quantum operations.

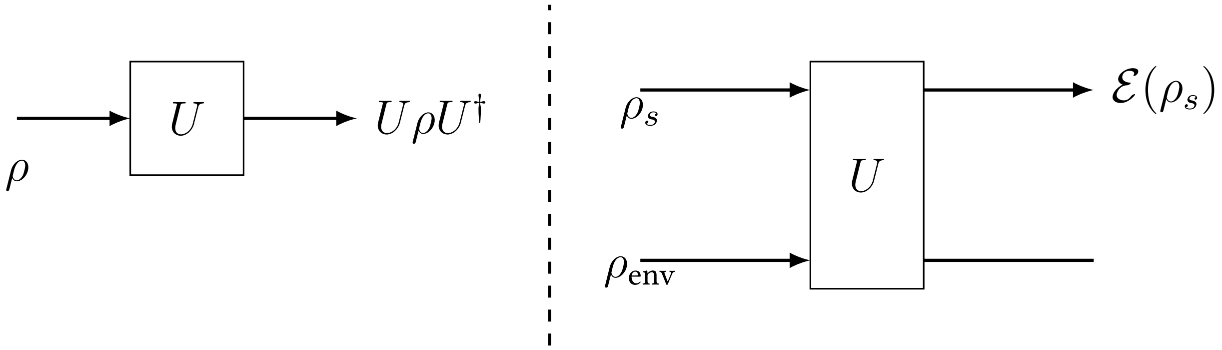

FIGURE A.1: Models of closed (left) and open (right) quantum systems. An open quantum system consists of two parts, the principal system and an environment.

Note that the map defined by $\mathcal{E}(\rho) = U\rho U^\dagger$ satisfies the properties of Definition 11, and thus the unitary evolution operation in closed systems is a quantum channel. On the other hand, in open systems, the general state is the coupling between the system and the environment, i.e., $\rho = \rho_s \otimes \rho_{env}$, where $\rho \in \mathcal{L}(\mathcal{H}^s) \otimes \mathcal{L}(\mathcal{H}^{env})$. However, our interest is restricted to how the state of the principal system evolves. In this sense, we can obtain this evolved state by taking the partial trace, with respect to the environment, over the state ρ evolved under the unitary U that acts on both the system and the environment. Indeed, this defines the quantum channel $\mathcal{E}$ as:

$$\begin{aligned} \mathcal{E} : \mathcal{L}(\mathcal{H}^s) \otimes \mathcal{L}(\mathcal{H}^{env}) &\rightarrow \mathcal{L}(\mathcal{H}^s) & \text{(A.4)} \\ \rho = \rho_s \otimes \rho_{env} &\rightarrow \mathcal{E}(\rho) = \mathrm{Tr}_{env}\left\{U\rho U^\dagger\right\} = \mathrm{Tr}_{env}\left\{U(\rho_s \otimes \rho_{env})U^\dagger\right\} & \text{(A.5)} \end{aligned}$$

The expression above in Eq. (A.5) defines, in general, the evolution of a quantum state. In particular, if there is no environment in the description of the complete system, then the general state is $\rho = \rho_s$, and the unitary can be identified as U_s, which acts only on the Hilbert space of the principal system. Thus, the partial trace over the environment is trivial, and we are left with:

$$\mathcal{E}(\rho) = \mathrm{Tr}_{env}\left\{U\rho U^\dagger\right\} = \mathrm{Tr}_{env}\left\{U_s\rho_s U_s^\dagger\right\} = U_s\rho_s U_s^\dagger,$$

which is the limiting case of a closed system.

On the other hand, in the case of an open system, we can develop Expression (A.5). To do so, suppose that the environment state is given by $\rho_{env} = |\psi_{env}\rangle\langle\psi_{env}|$, and let $\{e_k\}$ be an orthonormal basis of the environment's Hilbert space. Moreover, any unitary U defined on the space $\mathcal{H}^s \otimes \mathcal{H}^{env}$ can be written as $U = \sum_\mu U_\mu^s \otimes U_\mu^{env}$. With this, we have the following development:

$$\begin{aligned} \mathcal{E}(\rho) &= \mathrm{Tr}_{env}\left\{U(\rho_s \otimes \rho_{env})U^\dagger\right\} \\ &= \sum_k (\mathbb{1}_s \otimes \langle e_k|)\left[\left(\sum_\mu U_\mu^s \otimes U_\mu^{env}\right)(\rho_s \otimes |\psi_{env}\rangle\langle\psi_{env}|)\left(\sum_\nu U_\nu^{s\,\dagger} \otimes U_\nu^{env\,\dagger}\right)\right](\mathbb{1}_s \otimes |e_k\rangle) \\ &= \sum_k (\sum_{\mu,\nu} \langle e_k| U_\mu^{env} |\psi_{env}\rangle \ (U_\mu^s \rho_s U_\nu^{s\,\dagger}) \ \langle\psi_{env}| U_\nu^{env\,\dagger} |e_k\rangle \\ &= \sum_k \left(\sum_\mu \langle e_k| U_\mu^{env} |\psi_{env}\rangle U_\mu^s\right) \rho_s \left(\sum_\nu U_\nu^{s\,\dagger} \langle\psi_{env}| U_\nu^{env\,\dagger} |e_k\rangle\right) \end{aligned}$$

Then, the operator $E_k : \mathcal{H}^{env} \rightarrow \mathcal{H}^s$ is defined, where for each $|e_k\rangle$, the operator E_k is associated by:

$$E_k \equiv \sum_\mu \langle e_k| U_\mu^{env} |\psi_{env}\rangle U_\mu^s = \langle e_k|U|\psi_{env}\rangle \tag{A.6}$$

which acts on the principal system. Note that the inner product appearing in the second equality of Eq. (A.6) is the partial inner product, which acts only on the part of the unitary U that operates on the Hilbert space $\mathcal{H}^{env}$. Indeed, the operators E_k are called sum operators, (super)operators of Kraus, or simply Kraus operators. Thus, the most general evolution in a quantum system is described as:

$$\mathcal{E}(\rho) = \sum_k E_k \rho_s E_k^\dagger. \tag{A.7}$$

In particular, the set of Kraus operators $\{E_k\}$ forms a complete set only if the quantum channel $\mathcal{E}$ is trace-preserving. Indeed, observe that by taking the trace of $\mathcal{E}(\rho)$, we have:

$$1 = \mathrm{Tr}\{\mathcal{E}(\rho)\} = \mathrm{Tr}\left\{\sum_k E_k \rho_s E_k^\dagger\right\} = \mathrm{Tr}\left\{\left(\sum_k E_k E_k^\dagger\right)\rho_s\right\} \implies \sum_k E_k E_k^\dagger = \mathbb{1}_s \tag{A.8}$$

since the above equality must hold for every state ρ, this implies that the operator $\sum_k E_k E_k^\dagger$ must necessarily be the identity operator. In the general scenario, where $\mathcal{E}$ is not trace-preserving, we have:

$$\mathrm{Tr}\{\mathcal{E}(\rho)\} \leq 1 \implies \mathrm{Tr}\left\{\left(\sum_k E_k E_k^\dagger\right)\rho_s\right\} \leq 1 \implies \sum_k E_k E_k^\dagger \leq \mathbb{1}_s \tag{A.9}$$

where the result follows from the same argument as before. The previous inequality is defined in the matrix sense, where for given matrices A and B of the same order, we say that $A \leq B \iff u^T(B-A)u \geq 0$ for all vectors u correctly defined with respect to the order of A and B, i.e., $(B-A)$ is a non-negative operator.

In particular, the representation of the quantum channel $\mathcal{E}$ obtained in Eq. (A.7) is called the **Operator-Sum Representation**. Moreover, note that starting from the sum representation and assuming that the set of Kraus operators is such that Eq. (A.9) holds, it is possible to show that $\mathcal{E}$ satisfies all the axioms $A1$, $A2$, and $A3$. Indeed, $\mathcal{E}$ is linear, and thus the convexity imposed by $A2$ is immediately satisfied. On the other hand, since Eq. (A.9) holds, it follows that the positivity of the map $\mathcal{E}$ is achieved, because:

$$\sum_k E_k E_k^\dagger \leq \mathbb{1}_s \implies \mathrm{Tr}\{\mathcal{E}(\rho)\} = \mathrm{Tr}\left\{\sum_k E_k E_k^\dagger \rho\right\} \leq \mathrm{Tr}\left\{\rho\right\} = 1 \tag{A.10}$$

which shows that $\mathrm{Tr}\{\mathcal{E}(\rho)\} \leq 1$. On the other hand,

$$\mathrm{Tr}\{\mathcal{E}(\rho)\} = \mathrm{Tr}\left\{\sum_k E_k E_k^\dagger \rho\right\} = \sum_k \mathrm{Tr}\left\{E_k^\dagger \rho E_k\right\} \geq 0, \tag{A.11}$$

since every density operator ρ is positive. With this, axiom $A3$ is verified, and together with the previous inequality, we have that axiom $A1$ is also verified. Thus, the sum representation satisfies all the axioms $A1$, $A2$, and $A3$.

However, it is also possible to show that any quantum channel that satisfies all the axioms

$A1$, $A2$, and $A3$ must necessarily be expressed as a sum representation. The proof is simple; to do so, let us define the general state $|\alpha\rangle = \sum_i |i_s\rangle \otimes |i_{env}\rangle$. Furthermore, let us define the operator σ in the space $\mathcal{H}^s \otimes \mathcal{H}^{env}$ as:

$$\sigma \equiv (\mathbb{1}_{env} \times \mathcal{E})(|\alpha\rangle \langle\alpha|) \tag{A.12}$$

where $\mathcal{E}$ is a quantum channel. We will show that $\mathcal{E}$ admits an operator-sum representation. To do so, let us take the state $|\psi\rangle = \sum_j \psi_j |j_s\rangle$ in the principal system and the corresponding $|\tilde{\psi}\rangle \equiv \sum_j \psi_j^* |j_{env}\rangle$ in the environment. Then, observe that:

$$\langle\tilde{\psi}|\sigma|\tilde{\psi}\rangle = \langle\tilde{\psi}| \left(\sum_{ij} |i_{env}\rangle \langle j_{env}| \otimes \mathcal{E}\left(|i_s\rangle \langle j_s|\right) \right) |\tilde{\psi}\rangle = \sum_{ij} \psi_i \psi_j^* \mathcal{E}\left(|i_s\rangle \langle j_s|\right) = \mathcal{E}(|\psi\rangle\langle\psi|)$$

which follows from the convexity of $\mathcal{E}$. Now, let $\sigma = \sum_i |s_i\rangle \langle s_i|$ be some decomposition of σ, where the vectors $|s_i\rangle$ need not be normalized. Let us define the map $E_i(|\psi\rangle) \equiv \langle\tilde{\psi}|s_i\rangle$, which gives us the following development:

$$\sum_i E_i |\psi\rangle \langle\psi| E_i^\dagger = \sum_i \langle\tilde{\psi}|s_i\rangle \langle s_i|\tilde{\psi}\rangle = \langle\tilde{\psi}| \sigma |\tilde{\psi}\rangle = \mathcal{E}(|\psi\rangle \langle\psi|). \tag{A.13}$$

Therefore, we obtain::

$$\mathcal{E}(|\psi\rangle \langle\psi|) = \sum_i E_i |\psi\rangle \langle\psi| E_i^\dagger \tag{A.14}$$

for all pure states, $|\psi\rangle$, of $\mathcal{H}^f$. By convex-linearity it follows that

$$\mathcal{E}(\rho) = \sum_i E_i \rho E_i^\dagger \tag{A.15}$$

In general, the condition $\sum_i E_i^\dagger E_i \leq I$ follows immediately from **Axiom A1**, which identifies the trace of $\mathcal{E}(\rho)$ with a probability. This demonstrates that the axiomatic representation implies the sum representation. Furthermore, combined with the previous result, we establish the equivalence between the axiomatic and operator-sum representations.

Thus, any set of quantum operations must be characterized by a set of Kraus operators $\{E_k\}$. However, a natural question that arises in this context concerns the uniqueness of the Kraus operators, i.e., can a quantum operation $\mathcal{E}$ be described by only one unique set of Kraus operators $\{E_k\}$? Indeed, the answer to this question is no. In fact, the Kraus operators are defined in such a way that there is an inherent redundancy in their definition, which allows for their non-uniqueness. Given the importance of this result, let us state it as a theorem below.

Theorem 8. *(Unitary freedom in the operator-sum representation [41]) Suppose* $\{E_1, \dots, E_m\}$ *and*

$\{F_1, \ldots, F_n\}$ are operation elements giving rise to quantum operations $\mathcal{E}$ and $\mathcal{F}$, respectively. By appending zero operators to the shorter list of operation elements we may ensure that $m = n$. Then $\mathcal{E} = \mathcal{F}$ if and only if there exist complex numbers u_{ij} such that $E_i = \sum_j u_{ij} F_j$, and u_{ij} is an m by m unitary matrix.

Proof. To begin, consider two quantum states $|\psi_i\rangle$ and $|\psi_j\rangle$. It is well known that these states generate the same density operator if and only if they are related by:

$$|\psi_i\rangle = \sum_j u_{ij} |\varphi_j\rangle ,$$

where u_{ij} is a unitary matrix of complex numbers. If the states have different dimensions, we use a trivial embedding between the Hilbert spaces such that they are completed with zeros until both have the same dimension.

Now, suppose that $\{E_i\}$ and $\{F_j\}$ are two sets of operation elements for the same quantum operation, satisfying $\sum_i E_i \rho E_i^\dagger = \sum_j F_j \rho F_j^\dagger$ for all ρ. We define the following states:

$$|e_i\rangle \equiv \textstyle\sum_k |k_R\rangle (E_i |k_Q\rangle) , \quad |f_j\rangle \equiv \displaystyle\sum_k |k_R\rangle (F_j |k_Q\rangle) . \tag{A.16}$$

Now, using the definition of the operator σ introduced in Eq. (A.12), it follows that $\sigma = \sum_i |e_i\rangle \langle e_i| = \sum_j |f_j\rangle \langle f_j|$, and thus there exists a unitary matrix u_{ij} such that

$$|e_i\rangle = \sum_j u_{ij} |f_j\rangle . \tag{A.17}$$

For an arbitrary state $|\psi\rangle$, we have

$$E_i |\psi\rangle = \langle \tilde{\psi} | e_i \rangle = \sum_j u_{ij} \langle \tilde{\psi} | f_j \rangle = \sum_j u_{ij} F_j |\psi\rangle \implies E_i = \sum_j u_{ij} F_j . \tag{A.18}$$

Conversely, assuming that E_i and F_j are related by a unitary transformation of the form $E_i = \sum_{ij} u_{ij} F_j$, we can show that the Kraus operators $\{E_i\}$ generate the same quantum operation as the operators $\{F_j\}$. Indeed, consider a given E_i:

$$E_i \rho E_i^\dagger = \left(\sum_{ij} u_{ij} F_j \right) \rho \left(\sum_{ik} u_{ik}^\dagger F_k^\dagger \right) = \sum_{jk} \left(\sum_i u_{ij} u_{ik}^\dagger \right) F_j \rho F_k^\dagger = \sum_{jk} \delta_{jk} F_j \rho F_k^\dagger = F_j \rho F_j^\dagger .$$

This implies that, for each specific index i, the operation $E_i \rho E_i^\dagger$ is equivalent to an operation at a specific index j. Summing over all indices i, we obtain:

$$\mathcal{E}(\rho) = \sum_i E_i \rho E_i^\dagger = \sum_j F_j \rho F_j^\dagger .$$

Thus, the equivalence between the quantum operations is established. □

The formalism of quantum channels is fundamentally rich. Indeed, the previous developments lay the foundation for several other particularly interesting results associated with quantum channels. To illustrate one such application, we will present the measurement model. In essence, the measurement model consists of constructing a measurement scheme based on a set of trace-preserving Kraus operators $\{E_m\}$.

In this context, for each m, let E_{mk} be a set of operation elements for $\mathcal{E}_m$. Introduce an environmental system E, with an orthonormal basis $|m, k\rangle$ in one-to-one correspondence with the set of indices for the operation elements. Analogously to the earlier construction, define an operator U such that

$$U|\psi\rangle\,|e_0\rangle = \sum_{mk} E_{mk}|\psi\rangle|m,k\rangle.$$

Then, given $P_m = \sum_k |m,k\rangle\,\langle m,k|$ as a projector onto the environment, the measurement with P_m yields:

$$\begin{aligned}
\mathrm{Tr}\left\{P_m U\left[\rho\otimes|e_0\rangle\,\langle e_0|\right]U^\dagger\right\} &= \mathrm{Tr}\left\{P_m\sum_\alpha p_\alpha U\left(|\psi_\alpha\rangle\,\langle\psi_\alpha|\otimes|e_0\rangle\,\langle e_0|\right)U^\dagger\right\}\\
&= \mathrm{Tr}\left\{P_m\sum_\alpha p_\alpha U\,|\psi_\alpha\rangle\,|e_0\rangle\left(U\,|\psi_\alpha\rangle\,|e_0\rangle\right)^\dagger\right\}\\
&= \mathrm{Tr}\left\{\sum_{\substack{\alpha,m,k,\\ k',r,t'}} p_\alpha E_{mk'}E^\dagger_{rt}\,|\psi_\alpha\rangle\,\langle\psi_\alpha|\,\delta_{k,k'}\delta_{m,r}\delta_{k,t}\delta_{mm'}\right\}\\
&= \mathrm{Tr}\left\{\sum_{\alpha,k} p_\alpha E_{mk}E^\dagger_{mk}\,|\psi_\alpha\rangle\,\langle\psi_\alpha|\right\}\\
&= \mathrm{Tr}\left\{\sum_k E_{mk}\left(\sum_\alpha p_\alpha\,|\psi_\alpha\rangle\,\langle\psi_\alpha|\right)E^\dagger_{mk}\right\} = \mathrm{Tr}\left\{E_m(\rho)\right\}
\end{aligned}$$

With $\mathcal{E}(\rho) \equiv \sum_k E_{mk}\rho E^\dagger_{mk}$, this determines that the probability associated with the label m in a measurement is given by $\mathrm{Tr}\left\{E_m(\rho)\right\}$. Given this result, we see that, according to the measurement postulate, the post-measurement state $\tilde{\rho}$ can be written as:

$$\tilde{\rho} = \frac{P_m\left[U\left(\rho\otimes|e_0\rangle\,\langle e_0|\right)U^\dagger\right]P_m}{\mathrm{Tr}\left\{P_m U\left[\rho\otimes|e_0\rangle\,\langle e_0\right]\right.} = \frac{\mathcal{E}_m(\rho)}{\mathrm{Tr}\left\{\mathcal{E}_m(\rho)\right\}}. \tag{A.19}$$

which establishes the result of how the measurement postulate in quantum mechanics is expressed in terms of a quantum operation.

Furthermore, there are other common models of quantum channels, which we state and briefly highlight their applications below.

- **Partial trace.** The partial trace is a quantum channel that acts on a composite system ρ_{AB}, tracing out one of the subsystems (for example, B) and resulting in a reduced state on subsystem A:

  $$\mathcal{E}_{\mathrm{tr}_B}(\rho_{AB}) = \mathrm{tr}_B(\rho_{AB}).$$

  The Kraus operators for the partial trace over B are:

  $$E_i = \mathbb{1}_A \otimes \langle b_i| \,,$$

  where $\{|b_i\rangle\}$ is an orthonormal basis for subsystem B.

- **Bit-flip Channel.** The bit-flip channel performs a bit flip on the state $|0\rangle$ of the computational basis to the state $|1\rangle$, also in the computational basis. Indeed, this quantum channel is characterized by the following Kraus operators:

  $$E_0 = \sqrt{p}\mathbb{1} = \sqrt{p}\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad E_1 = \sqrt{1-p}\sigma_x = \sqrt{1-p}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}.$$

- **Phase-flip Channel.** The phase-flip channel introduces quantum phase errors through the action of the Pauli matrix σ_z with probability $1-p$. Furthermore, the phase flip does not modify the populations of the quantum state. The Kraus operators characterizing the phase-flip channel are:

  $$E_0 = \sqrt{p}\mathbb{1} = \sqrt{p}\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad E_1 = \sqrt{1-p}\sigma_z = \sqrt{1-p}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

- **Depolarizing Channel.** The depolarizing channel is a quantum channel that models the addition of quantum noise, where the state ρ is mixed with the maximally mixed state $\frac{\mathbb{1}}{d}$, assigning a probabilistic weight $p \in [0,1]$. Specifically, the depolarizing channel is represented by:

  $$\mathcal{E}(\rho) = \frac{p\mathbb{1}}{2} + (1-p)\rho.$$

- **Amplitude Damping.** The amplitude damping channel is a model of quantum noise that describes the loss of energy from a quantum system to the environment, as occurs, for example, in spontaneous decay or relaxation processes. This channel is particularly relevant for physical systems such as atoms, ions, or quantum circuits, where energy dissipation is common. The amplitude damping channel can be represented by the following Kraus operators:

$$E_0 = \begin{bmatrix} 1 & 0 \\ 0 & \sqrt{1-\gamma} \end{bmatrix}, \quad E_1 = \begin{bmatrix} 0 & \sqrt{\gamma} \\ 0 & 0 \end{bmatrix},$$

where γ denotes the probability of decay from an excited state $|1\rangle$ to the ground state $|0\rangle$.

- **Phase Damping.** The phase damping channel is a model of quantum noise that affects the relative phases between states in a superposition without altering the populations of the states. It is described by the Kraus operators:

$$E_0 = \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{1-\lambda} \end{pmatrix}, \quad E_1 = \begin{pmatrix} 0 & 0 \\ 0 & \sqrt{\lambda} \end{pmatrix},$$

where λ is the probability of coherence loss.

Indeed, the quantum channels presented above constitute the main quantum channels employed in the context of quantum information theory. However, there are some particular results that are obtained especially for certain channels possessing specific properties. In particular, for the regime of Markovian dynamics, it is possible to show that the formalism of quantum channels leads to the Lindblad equation for open systems [41].

In the specific context of our work, the quantum channel described by quantum twirling is a unital quantum channel, that is, $\mathcal{E}(\mathbb{1}) = \mathbb{1}$, and furthermore, it is a conditional expectation quantum channel, which we define below.

Definition 12. *(Conditional expectation of quantum channel [134]). The map* $\Lambda : \mathcal{L}(\mathcal{H}^{d_1}) \to \mathcal{L}(\tilde{\mathcal{H}}^{d_2})$ *where* $\mathcal{H}^{d_1}$ *and* $\tilde{\mathcal{H}}^{d_2}$ *are a* d_1,d_2*-dimensional Hilbert space which satisfies:*

(i) Λ *is a positive map,*

(ii) $\Lambda(B) = B$ *for all* $B \in \mathcal{L}(\tilde{\mathcal{H}}^{d_2})$,

(iii) $\Lambda(AB) = \Lambda(A)B$ *for all* $A \in \mathcal{L}(\mathcal{H}^{d_1})$ *and all* $B \in \mathcal{L}(\tilde{\mathcal{H}}^{d_2})$,

(iv) Λ *is trace preserving.*

is called a conditional expectation.

Certainly, it is easy to verify that the operator $\Lambda_{\mathcal{G}_\mathrm{T}}$ is a particular case of a conditional expectation because, as we defined in Chapter 3, $\mathcal{L}(\tilde{\mathcal{H}}^d)$ corresponds to the subspace of density operators that are invariant under the action of the thermodynamic group.

In our work, a particular result of interest is the guarantee that the splitting of gauge entropy into diagonal entropy plus Holevo asymmetry is valid, and that the Holevo asymmetry is zero if and only if the Hamiltonian has no degeneracies (provided that the state ρ is non-invariant). Indeed, this result is achieved by employing the Data Processing Inequality on the well-known Kullback-Leibler divergence, which we define below.

Definition 13. *(Kullback-Leibler divergence [50]). Let p be a probability distribution defined on the alphabet $\mathcal{X}$, and let $q : \mathcal{X} \to [0, \infty)$. The relative entropy $D(p\|q)$ is defined as follows:*

$$D(p\|q) \equiv \begin{cases} \sum_x p(x) \log \left[\dfrac{p(x)}{q(x)}\right] & \textit{if } \operatorname{supp}(p) \subseteq \operatorname{supp}(q), \\ +\infty & \textit{else}, \end{cases}$$

where $\operatorname{supp}(\cdot)$ *denotes the support of the argument.*

In particular, it is worth noting that the Kullback-Leibler divergence is not a metric in the usual (mathematical) sense. Specifically, it can be shown that the triangle inequality does not hold for this map. However, it can still be used as a measure of information and similarity between two probability distributions p and q, with its application relating to how similar these two distributions are in terms of their entropic content, given by the Shannon entropy (classical case) and von Neumann entropy (quantum case).

Finally, we state the Data Processing Inequality, which constitutes a fundamental result in quantum information theory.

Theorem 9. *(Data processing inequality). Given $\Lambda : \mathcal{A} \to \mathcal{N}$ a conditional expectation and two positive states $\rho, \sigma \in \mathcal{A}$, the following inequality holds*

$$D(\rho\|\sigma) \geq D(\Lambda(\rho)\|\Lambda(\sigma)) \tag{A.20}$$

and the equality holds if, and only if,

$$\rho = \sigma^{1/2}\sigma_{\mathcal{N}}^{-1/2}\rho_{\mathcal{N}}\sigma_{\mathcal{N}}^{-1/2}\sigma^{1/2}. \tag{A.21}$$

Proof. For inequality in (A.20) see Ref. [135]. The result associated with the necessary and sufficient conditions for equality in (A.20) to be achieved can be found in Ref [134]. ☐

Appendix B

Group theory and Haar average

Some definitions from group theory and Lie groups are presented. In addition, the general result for Haar averages over the unitary group is obtained.

B.1 Group theory and Lie groups

Definition 14. *(Group) A group is a tuple $(G, \cdot)$ where G is a non-empty set and $\cdot$ is a operation, which we call the product, defined by:*

$$\begin{aligned} \cdot : G \times G &\rightarrow G \\ (a, b) &\rightarrow c = a \cdot b, \end{aligned} \tag{B.1}$$

where a, b and c are elements on G. And the product operation satisfies the following properties:

- *$a \cdot (b \cdot c) = (a \cdot b) \cdot c$ for all $a, b, c \in G$. I.e. the product operation is associativity,*
- *There exists an element $k \in G$ such that: $a \cdot k = a$ for all $a \in G$. In special, k is called identity element on G,*
- *For very element $a \in G$ exists an element $b \neq a$ such that $a \cdot b = b \cdot a = k$. The element b is called inverse of a and is usually denoted by $b = a^{-1}$.*

For simplicity, we will refer to the group simply as G, omitting the notation $(G, \cdot)$, but making it clear that the group structure is formed by the tuple of a non-empty set and an operation called product as per Definition 14.

Definition 15. *(Abelian group) If G is a group equipped with the product operation, and this operation is commutative, i.e., the following equality holds:*

$$a \cdot b = b \cdot a \tag{B.2}$$

for all $a, b \in G$, then G is called abelian group. However, if this property not holds, we call G as non-abelian group.

Definition 16. *(Finite group) The group G is called finite when the set G is finite. Therefore, G is infinite when G not is finite.*

In our work, we are interested in a specific type of groups, which are called Lie groups. In fact, Lie groups differ from groups defined only according to Definition 14. In summary, Lie groups possess an intrinsically geometric and topological character due to being defined under a specific type of mathematical structure known as manifolds. Thus, we will briefly introduce the notion of differentiable manifolds, and shortly thereafter, we will connect it with the structure of groups.

Definition 17. *(Diferential manifold [136]) Let us consider a non-empty set G with a distinguished family of open subsets with the following properties:*

- *I) the empty set and the set G are both open,*
- *II) the intersection of any finite collection of open sets is again open,*
- *III) the union of any collection (enumerable) of open sets is again open.*

Furthermore,

- *IV) G is provided with a family of pairs $\{(U_i, \varphi_i)\}$;*
- *V) U_i is a family of open sets which covers G, that is, $\bigcup_i U_i = G$ where φ_i is a homeomorphism from U_i onto an open subset U_i' of $\mathbb{R}^m$.*
- *VI) given U_i and U_j such that $U_i \cap U_j \neq \emptyset$, the map $\psi_{ij} = \varphi_i \circ \varphi_j^{-1}$ from $\varphi_j(U_i \cap U_j)$ to $\varphi_i(U_i \cap U_j)$ is infinitely differentiable.*

If G satisfies properties I, II, and III, then G is said to be a topological space. If G is a topological space that satisfies properties IV, V, and VI, then G is said to be a differentiable manifold. In summary, properties I, II, and III of Definition 17 introduce a topological structure to the set G; consequently, notions of distance and measure can be constructed on this set based on that. Moreover, properties IV, V, and VI introduce generality regarding the topology of the set G. However, the introduction of the homeomorphism constructed from the open sets U_i of G with the open sets U_i' of $\mathbb{R}^m$ allows a manifold to be locally mapped into a subset of $\mathbb{R}^m$. Finally, item VI introduces the map ψ that connects two topological descriptions made from different open sets of the manifold, allowing for coordinate changes.

Requiring the differentiability of the manifold G enables us to bring usual calculus concepts into this set. With this framework in place, we can finally obtain the elegant notion of a Lie group and Compact Lie group.

Definition 18. *(Lie group) A Lie group is a smooth manifold G equipped with an operation called multiplication, such that the elements of G satisfy it as in the Definition 14.*

With this, we already have an interesting mathematical structure; however, we still need to introduce an important concept to Lie groups that will allow us to have a vector space structure from our manifold (G).

Definition 19. *(Lie algebra) A Lie algebra $\mathfrak{g}$ associated with a group G is a vector space formed by the left-invariant vector fields X on G endowed with a product, called the Lie bracket or commutator $[\cdot,\cdot] : \mathfrak{g} \times \mathfrak{g} \to \mathfrak{g}$, which satisfies the following properties:*

I) Bilinearity, i.e., linear in each argument.

II) Anti-symmetry, that is, $[X, Y] = -[Y, X]$ for all $X, Y \in \mathfrak{g}$.

III) The Jacobi identity, that is, for all $X, Y, Z \in \mathfrak{g}$, we have

$$[X, [Y, Z]] + [Z, [X, Y]] + [Y, [Z, X]] = 0. \tag{B.3}$$

Definition 20 (Compact Lie Group)**.** *A Lie group G is **compact** if and only if it For every collection $\{\mathcal{U}_\alpha\}_{\alpha \in I}$ of open sets in G (where I is an arbitrary index set) such that:*

$$G \subseteq \bigcup_{\alpha \in I} \mathcal{U}_\alpha \quad \textit{(open cover)} \tag{B.4}$$

*there exists a **finite** subset $J \subset I$ with:*

$$G \subseteq \bigcup_{\alpha \in J} \mathcal{U}_\alpha \quad \textit{(finite subcover).} \tag{B.5}$$

In particular, not all Lie groups are compact. Below we present some key examples:

Category	*Group*	*Description and Physical Relevance*
Compact	$\mathrm{SO}(n)$	Special orthogonal group (rotations in $\mathbb{R}^n$). Preserves Euclidean norm. Fundamental in rigid body dynamics.
	$\mathrm{SU}(n)$	Special unitary group (unitary matrices with det= 1). Core structure in quantum mechanics.
	$\mathrm{U}(1)$	Circle group (complex phases $e^{i\theta}$). Governs gauge transformations in QED.
	$\mathrm{Sp}(n)$	Compact symplectic group. Important in Hamiltonian mechanics.
Non-Compact	$\mathrm{GL}(n, \mathbb{R})$	General linear group (invertible $n \times n$ matrices). Basis for representation theory.
	$\mathrm{SL}(n, \mathbb{R})$	Special linear group (det= 1). Appears in fluid dynamics.
	$\mathrm{SO}(p, q)$	Indefinite orthogonal group. Preserves metric with signature (p, q). Used in relativity.
	Heis_3	Heisenberg group. Key in quantum harmonic oscillators.
	Poincaré	Poincaré group (isometries of spacetime). Fundamental in QFT.

A particularly interesting Lie bracket is the commutator, usually defined by $[A, B] = AB - BA$ for any $A, B \in \mathfrak{g}$. An interesting aspect is the relationship between a Lie group G and its algebra $\mathfrak{g}$. In fact, this connection can be made through the so-called exponential map [72, 75], which is formally defined by:

$$\begin{aligned} \exp : \mathfrak{g} &\rightarrow G && \text{(B.6)} \\ X \in \mathfrak{g} &\rightarrow g \equiv \exp(X) \in G && \text{(B.7)} \end{aligned}$$

Note that the exponential map is not necessarily equivalent to the exponential function; however, for matrix Lie groups, the notions become equivalent, and thus the elements of a group can be written as $g = e^X$. Furthermore, the elements $X \in \mathfrak{g}$ are called generators of the algebra.

B.2 Group Representation Theory

The mathematical structure provided by a Lie group—and consequently its manifold—is still not sufficient for constructing various important physical concepts, especially for defining vector spaces. However, from a Lie group, we can obtain a vector space.

Definition 21. *(Representations) A representation of a Lie group G is a pair (V, π), where V is a vector space, and $\pi : G \rightarrow \mathrm{GL}(V)$ is a linear G-action on V.*

To illustrate the concept of representation in a Lie group G, let us consider the group $G = SU(2)$, the special unitary group of dimension 2. In fact, the Lie algebra of the group is $\mathfrak{su}(2)$, whose generators are the Pauli matrices defined by:

$$\sigma_x = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_y = \frac{1}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_z = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{B.8}$$

which satisfy the following commutation relation that characterizes the algebra $\mathfrak{su}(2)$:

$$[\sigma_\alpha, \sigma_\beta] = \frac{\epsilon_{\alpha,\beta,\gamma}}{2}\sigma_\gamma. \tag{B.9}$$

where $\epsilon_{\alpha,\beta,\gamma}$ is the Levi-Civita tensor. Now, let us consider the following matrices:

$$J_x = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \quad J_y = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \quad J_z = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \tag{B.10}$$

In fact, it is not difficult to verify that the matrices defined in (B.10) have zero trace and satisfy the same type of commutation relation presented in Eq. (B.9). In summary, this simple example effectively illustrates the notion of a group's representation; indeed, the matrices J_α

represent the Lie algebra $\mathfrak{su}(2)$ in the space of 3×3 matrices. However, both sets in Eq. (B.8) and Eq. (B.10) represent the same algebra and are associated with the same group of transformations, SU(2), regardless of the dimension of the vector space for which the group is represented.

This small example leads us to important notions within representation theory. In this sense, we will introduce these concepts next, first defining the notion of G-morphisms or intertwiners.

Definition 22. *(morphism) Let $\pi_V : G \to V$ and $\pi_W : G \to W$ be two representations of G in the spaces V and W. A G-morphism ($G-$Homomorphism or intertwiners map) between them is a linear map $\varphi : V \to W$ such that*

$$\varphi(\pi_V(g) \cdot v) = \pi_W(g) \cdot \varphi(v) \tag{B.11}$$

for all $g \in G$ and $v \in V$.

With this, we can define the following types of representations.

Definition 23. *(Types of representations) Let $\pi : G \to GL(V)$ be a representation of a group G in the space of linear operators on a vector space V. Then, we say:*

(I) The representation π is trivial if for all $g \in G$, we have $\pi(g) = \mathbb{1}_V$,

(II) Consider a second representation of G in a space W, i.e., $\pi_W : G \to GL(W)$. Then, π and π_W are called equivalent representations if there exists a linear operator $A : V \to W$ such that:

$$A\pi(g) = \pi_W(g)A \tag{B.12}$$

for all $g \in G$.

Now, let us define invariant subspaces.

Definition 24. *(Invariant subspace) Consider the representation π_V of the group G in the vector space V. A subspace W of V is called an invariant subspace under the representation π_V if $\pi(g)w \in W$ for all $g \in G$, that is, $\pi(G)W \subset W$.*

Note that from the definition of invariant subspaces, it is immediate that any representation always has at least two invariant subspaces, which are:

- The first invariant space is formed by the zero vector $W = \{0\}$,
- The other invariant space is the entire space, i.e., $V = W$.

These two subspaces are referred to as trivial invariant subspaces or simply trivial subspaces.

The notion of invariant subspaces is substantially important within representation theory since it allows us to establish the notion of irreducible representations, which are formally defined as follows.

Definition 25. *(Irreducible representations) A representation π_V of a group G in a vector space V is said to be irreducible if its only invariant subspaces are trivial. If a representation is not irreducible, it is said to be reducible.*

In particular, both irreducible and reducible representations are interesting and relevant to the context of this work. Specifically, there is an interesting case concerning reducible representations that occurs when a space V can be decomposed into a direct sum of spaces V_k, i.e., $V = \bigoplus_{k=1}^{p} V_k$, where each subspace V_k is invariant. Under these circumstances, we can write the representation π_V as:

$$\pi_V(g) = \begin{pmatrix} \pi_{V_1}(g) & & \\ & \ddots & \\ & & \pi_{V_p}(g) \end{pmatrix} \tag{B.13}$$

for all $g \in G$, where each representation π_{V_k} acts on a subspace V_k. When all the representations π_{V_k} are irreducible, we say that the representation $\pi_V(g)$ is a maximally/completely reducible representation.

In the context of operators, given an irreducible representation of some subspace π_{V_k}, it follows that the set of operators $A : V_k \to V_k$ in this subspace such that:

$$\pi_{V_k}(g)A = A\pi_{V_k}(g) \tag{B.14}$$

for all $g \in G$ are of the form $A = \lambda \mathbb{1}_{V_k}$ for some $\lambda \in \mathbb{C}$. This result is demonstrated in Schur's Lemma in the following section.

B.3 Haar measure

In this section, we finally enter the context of Haar integration. In fact, the conception of a measure associated with groups—in our particular objective of compact Lie groups—is a generalization of the Lebesgue measure that we presented in Definition 9.

Theorem 10. *(Haar [137]) Let G be a compact group. Then, there exists a unique positive and normalized measure $\mathrm{d}\mu$ which is left and right invariant under the action of the group G. Therefore, for any integrable function, we have:*

$$\int_G \mathrm{d}\mu(g) f(g) = \int_G \mathrm{d}\mu(g) f(hg) = \int_G \mathrm{d}\mu(g) f(gh) = \int_G \mathrm{d}\mu(g) f(g^{-1}) \tag{B.15}$$

for all $h \in G$.

Proof. See Chapter 3 of [72] for a detailed discussion □

The positivity of the Haar measure implies, form some $g \in G$

$$\int_G d\mu(g)f(g) \geq 0 \implies \int_G d\mu(g)f(g) = 0 \implies f(g) = 0 \tag{B.16}$$

since $f \geq 0$. The normalization of Haar measure is:

$$\int_G d\mu(g) = 1. \tag{B.17}$$

Certainly, our interest is to ensure that the formalism introduced in Chapter 3 is fully valid. In this sense, the notion of Haar measure and integral must be extended to a multidimensional context. Indeed, this can be done formally by the Fubini Theorem, which we state in Theorem 7.

With this, we finally obtain the result that ensures the existence of the Haar measure, as we initially mentioned in Chapter 3. Furthermore, this result then establishes the foundation for the existence of the induced Haar measure of the gauge group in Eq. (3.28), which is given by Eq. (3.31), since for each instant t, the gauge group is always the Cartesian product of unitary groups (which are compact Lie groups) and, consequently, is a compact Lie group.

Next, we will develop the necessary methods to rigorously obtain the Haar average result given by Eq. (3.37). To do this, the first result we need to obtain is the so-called Schur's Lemma.

Lemma 1. *(Schur's Lemma) Let π_V and π_W be irreducible representations of a Lie group G in the spaces V and W. Consider the $G-$morphism $\varphi : V \to W$, then we have the following implications:*

(a) The G-morphism is either identically null or an isomorphism.

(b) If $V = W$, then $\varphi = \lambda \mathbb{1}$ for some $\lambda \in \mathbb{C}$.

Proof. First, we will demonstrate item (a). We can show that the sets $\mathrm{Ker}(\varphi)$ and $\mathrm{Im}(\varphi)$ are G-invariant subspaces of π_V and π_W. Indeed, note that given $x \in \mathrm{Ker}(\varphi)$, we have:

$$\varphi(\pi_V \cdot x) = \pi_W(g) \cdot \varphi(x) = \pi_W(g) \cdot 0 = 0 \tag{B.18}$$

for all $g \in G$. Then, $\pi_V(g)x \in \mathrm{Ker}(\varphi)$ for all $g \in G$, therefore $\mathrm{Ker}(\varphi)$ is invariant under π_V. On the other hands, for some $y \in \mathrm{Im}(\varphi)$ exist x such that

$$\varphi(\pi_V \cdot x) = \pi_W(g) \cdot \varphi(x) = \pi_W(g) \cdot y \tag{B.19}$$

for all $g \in G$. Then, $\pi_W(g)y \in \mathrm{Im}(\varphi)$, therefore $\mathrm{Im}(\varphi)$ is invariant under π_W.

Since π_V and π_W are irreducible representations, then your only invariant subspaces are the trivial subspaces, therefore, it follows that there are four possibilities to consider:

$$\mathrm{Ker}(\varphi) = V \quad e \quad \mathrm{Im}(\varphi) = W. \tag{B.20}$$

$$\mathrm{Ker}(\varphi) = \{0\} \quad e \quad \mathrm{Im}(\varphi) = W. \tag{B.21}$$

$$\mathrm{Ker}(\varphi) = V \quad e \quad \mathrm{Im}(\varphi) = \{0\}. \tag{B.22}$$

$$\mathrm{Ker}(\varphi) = \{0\} \quad e \quad \mathrm{Im}(\varphi) = \{0\}. \tag{B.23}$$

Note that the cases presented by Eq. (B.20) and Eq. (B.23) are impossible; indeed, both cases violate the Rank-Nullity Theorem. The cases (B.21) and (B.22) may occur, and if (B.21) occurs, then it follows that φ is an isomorphism from V to W. On the other hand, if (B.22) occurs, then the application φ is identically zero.

Now, we will prove item (b). Indeed, if $V = W$, then from item (a) of the Lemma, it follows that φ is either the zero map; in this case, we only need to take $\lambda = 0$, and the result is demonstrated, or the application is an isomorphism. Let us consider φ as an isomorphism; thus, it follows that for some $\lambda \in \mathbb{C}$, we have $p(\lambda) \equiv \varphi - \lambda\mathbb{1} = 0$, since λ is the eigenvalue of φ. Therefore, let us take $\mathrm{Ker}(p(\lambda))$, which is non-empty since the characteristic polynomial $p(\lambda)$ has some root in $\mathbb{C}$. Since $\mathrm{Ker}(\varphi - \lambda\mathbb{1})$ is non-empty, it follows that $\varphi - \lambda\mathbb{1}$ is not an isomorphism, according to item (a) of the Lemma; that is, the application $p(\lambda)$ is identically zero, hence it follows that:

$$p(\lambda) = 0 \implies \varphi - \lambda\mathbb{1} = 0 \implies \varphi = \lambda\mathbb{1} \tag{B.24}$$

as desired. □

B.3.1 Haar average over the unitary group

The Schur Lemma plays a unique role in determining Haar averages. In the context where G is a unitary group or a product of unitary groups, it is interesting to rewrite the Schur Lemma for this particular case [138]. In this sense, let us consider two finite-dimensional complex vector spaces $\mathcal{H}_{n_t^1}$ and $\mathcal{H}_{n_t^2}$ as $\mathbb{C}^{n_t^1}$ and $\mathbb{C}^{n_t^2}$, respectively, and let $G = \mathcal{U}(d)$.

Here, I introduced the notation with the label t. This index plays an important role in this work because we are in a context where, for each fixed instant of time t, we obtain a different group; furthermore, the label t can also be associated with a simple parameter that, in some way, modifies the studied group, as discussed in Chapter 5. Consequently, this notation is relevant for this work; however, if the reader is not in a similar context, it can and should be avoided to ensure simplicity and clarity in the notation.

Now, let us define the $G-$morphism between these two spaces, in this context this $G-$morphism are linear operators $A : \mathbb{C}^{n_t^1} \to \mathbb{C}^{n_t^2}$. Furthermore, the representations $v_t^1 : \mathcal{U}(d) \to \mathcal{H}_{n_t^1}$ and $v_t^2 : \mathcal{U}(d) \to \mathcal{H}_{n_t^2}$ are irreducible representations of the unitary group on $\mathbb{C}^{n_t^1}$ and $\mathbb{C}^{n_t^2}$.

From this, we see that G-morphism A is characterized by:

$$v_t^1 A = A v_t^2 \Longleftrightarrow v_t^1 A \left(v_t^2\right)^{-1} = A \Longleftrightarrow v_t^1 A \left(v_t^2\right)^{\dagger} = A. \tag{B.25}$$

With this in hand, we can now state Schur's Lemma for unitary groups, which we formalize below.

Lemma 2. *(Schur's Lemma for unitary group [138]) If* v_t^1 *and* v_t^2 *are irreducible representations of* $\mathcal{U}(d)$ *on* $\mathcal{H}_{n_t^1}$ *and* $\mathcal{H}_{n_t^2}$ *then:*

- *If* $n_t^1 \neq n_t^2$ *we have:*

$$v_t^1 A (v_t^2)^{\dagger} = A \implies A = \vec{0}. \tag{B.26}$$

- *If* $n_t^1 = n_t^2$ *and for equivalent* v_t^1 *and* v_t^2 *we have the following implication:*

$$v_t^1 A (v_t^2)^{\dagger} = A \implies A = \lambda \mathbb{1} \tag{B.27}$$

  where λ *is a constant.*

As mentioned, our goal is to formally derive the mathematical results that ensure the validity of the Haar average over a matrix X, as employed in this work. Specifically, we are interested in averages of the form:

$$X_{dd} = \int \mathrm{d}\mu \, \mathcal{V} X \mathcal{V}^{\dagger}, \;\; \mathcal{V} = \bigoplus_{k=1}^{p} v_t^k \tag{B.28}$$

where each $v_t^k \in \mathcal{U}(n_t^k)$, $\mathcal{V} \in \mathcal{U}(d)$ and the Haar measure is

$$\mathrm{d}\mu = \prod_{k=1}^{p} \mathrm{d}\mu_k, \;\; \mathrm{d}\mu_k = \mathrm{d}\mu[\mathcal{U}(n_t^k)]. \tag{B.29}$$

We now employ Schur's Lemma to derive an orthogonality relation associated with the irreducible representations v_t^k associated with each Hilbert subspace $\mathcal{H}_k$ of the Hilber space $\mathcal{H}_k$. To this end, we have the following Lemma.

Lemma 3. *(Orthogonality) Let* $\left\{v_t^k\right\}$ *be a family of non-equivalent irreducible representations of the unitary group on some complex vector spaces* $\mathcal{H}_k$ *and let* $\mathcal{H}^d = \bigoplus_{k=1}^{p} \mathcal{H}_k$. *Let* $X \in \mathcal{H}^d$ *be arbitrary* *linear operator on $\mathcal{H}^d$. Defining the trivial immersion of operators on $\mathcal{H}_k$ into operators on $\mathcal{H}^d$, $\mathcal{I}_k : \mathcal{H}_k \to \mathcal{H}^d$, by:*

$$\mathcal{I}_k(v_t^k) = \begin{cases} v_t^1 \oplus \left(\bigoplus_{m=1}^{p-1} \mathbb{0}_{n_m}\right), \ \textit{for}: \ k=1 \\ \left(\bigoplus_{m=1}^{k-1} \mathbb{0}_{n_m}\right) \oplus v_t^k \oplus \left(\bigoplus_{m=k+1}^{p} \mathbb{0}_{n_m}\right), \ \textit{for}: \ 1<k<p \\ \left(\bigoplus_{m=1}^{p-1} \mathbb{0}_{n_m}\right) \oplus v_t^p \ \textit{for}: \ k=p \end{cases} \tag{B.30}$$

for each $v_t^k \in \mathcal{H}_k$, where $\mathbb{0}_{n_m}$ are the $n_m \times n_m$ zero matrix.

Therefore, the averaging of X over all representations $\{v_t^k\}$ is diagonal in relation of the index k, i.e.

$$X_{dd} = \sum_{k,m} \int \mathrm{d}\mu \, \mathcal{I}_k(v_t^k) X \mathcal{I}_m(v_t^{m\dagger}) = \sum_k \int \mathrm{d}\mu_k \, \mathcal{I}_k(v_t^k) X \mathcal{I}_k(v_t^{k\dagger}). \tag{B.31}$$

Proof. Let consider the unitary representations $\tilde{v}_t^k$ and $\tilde{v}_t^m$ which are associated to the Hilbert subspace $\mathcal{H}_k$ and $\mathcal{H}_m$. Therefore, using the trivial immersion and considering the element k, q of the matrix X_{dd}, i.e.$(X_{dd})_{k,m}$, we have:

$$\begin{aligned} \mathcal{I}_k(\tilde{v}_t^k)\,(X_{dd})_{km}\,\mathcal{I}_m(\tilde{v}_t^{m\dagger}) &= \mathcal{I}_k(\tilde{v}_t^k)\left[\int \mathrm{d}\mu \, \mathcal{I}_k\left(v_t^k\right) X \mathcal{I}_m(v_t^{m\dagger})\right] \mathcal{I}_m(\tilde{v}_t^{m\dagger}) \\ &= \int \mathrm{d}\mu \, \mathcal{I}_k(\tilde{v}_t^k)\mathcal{I}_k(v_t^k) X \mathcal{I}_m(v_t^{m\dagger})\mathcal{I}_m(\tilde{v}_t^{m\dagger}) \\ &= \int \mathrm{d}\mu \, \mathcal{I}_k(\tilde{v}_t^k v_t^k) X \mathcal{I}_m(v_t^{m\dagger}\tilde{v}_t^{m\dagger}) \\ &= \int \mathrm{d}\mu \, \mathcal{I}_k(v_t^k) X \mathcal{I}_m(v_t^{m\dagger}) \end{aligned} \tag{B.32}$$

where the equality in Eq (B.32) follows from the left and right invariance of the Haar measure. Therefore, using the definition of $(X_{dd})_{q,m}$ we obtain the following equality:

$$\mathcal{I}_k(\tilde{v}_t^k)\,(X_{dd})_{km}\,\mathcal{I}_m(\tilde{v}_t^{m\dagger}) = (X_{dd})_{km}. \tag{B.33}$$

From Eq.(B.33), we obtain $k = m$. Indeed, we can identify the G-morphism as the matrix $(X_{dd})_{km}$. Thus, the G-equivariance property, together with Schur's Lemma, guarantees that $\mathcal{I}_k(\tilde{v}_t^k)$ and $\mathcal{I}_m(\tilde{v}_t^{m\dagger})$ are associated with isomorphic spaces, i.e., $\mathcal{H}_k \cong \mathcal{H}_{n_t^m}$. In particular, this implies $k = m$. Consequently, we find that the Haar average is diagonal in the index k, leading to the orthogonality relation for Haar averages, and Eq.(B.31) is obtained. □

We can now apply this orthogonality relation to evaluate the Haar average within each subspace. The following lemma summarizes this result.

Lemma 4. *(Haar average in subspace $\mathcal{H}_k$) Let v_t^k be an irreducible representation of the unitary group on some complex vector space $\mathcal{H}_k$ with dimension $\dim\{\mathcal{H}_k\} = n_t^k$. Let $X_t^k \in \mathcal{H}_k$ be arbitrary linear operator on $\mathcal{H}_k$. Then the Haar average of X_t^k over the unitary group $\mathcal{U}(n_t^k)$ are:*

$$[X_t^k]_{dd} = \int \mathrm{d}\mu_k \, v_t^k X_t^k v_t^{k\dagger} = \frac{\mathrm{Tr}\{X_t^k\}}{\dim\{\mathcal{H}_k\}} \mathbb{1}_{n_t^k} \tag{B.34}$$

where $\mathrm{d}\mu_k = \mathrm{d}\mu[\mathcal{U}(n_t^k)]$ and $\mathbb{1}_{n_t^k}$ is the identity operator in $n_t^k \times n_t^k$ dimension.

Proof. Let consider the unitary representation $\tilde{v}_t^k$ therefore, using the left and right invariance of the Haar measure, we have:

$$\begin{aligned}
\tilde{v}_t^k [X_t^k]_{dd} \tilde{v}_t^\dagger &= \tilde{v}_t^k \left(\int \mathrm{d}\mu_k \, v_t^k X_t^k v_t^{k\dagger} \right) \tilde{v}_t^\dagger \\
&= \int \mathrm{d}\mu_k (\tilde{v}_t^k v_t^k) X_t^k (v_t^{k\dagger} \tilde{v}_t^\dagger) \\
&= \int \mathrm{d}\mu_k \, v_t^k X_t^k v_t^{k\dagger} \\
&= [X_t^k]_{dd}
\end{aligned}$$

then, the equality is obtained:

$$\tilde{v}_t^k [X_t^k]_{dd} \tilde{v}_t^\dagger = [X_t^k]_{dd} \tag{B.35}$$

which holds for any unitary represetation $\tilde{v}_t^k$. Indeed, it follows from Schur's Lemma that the Haar average must be proportional to the identity operator. That is, we must have:

$$[X_t^k]_{dd} = C_t^k \mathbb{1}_{n_t^k}, \tag{B.36}$$

where C_t^k is the proportionality constant. We now determine the proportionality constant. Since the Haar average is proportional to the identity operator, it is diagonal. Therefore, its trace completely characterizes this operator. Evaluating the trace of the operator $[X_t^k]_{dd}$, we find that:

$$\begin{aligned}
\mathrm{Tr}\{[X_t^k]_{dd}\} &= \mathrm{Tr}\left\{\int \mathrm{d}\mu_k \, v_t^k X_t^k v_t^{k\dagger}\right\} \\
&= \sum_\alpha \langle\alpha| \left(\int \mathrm{d}\mu_k \, v_t^k X_t^k v_t^{k\dagger}\right) |\alpha\rangle \\
&= \sum_\alpha \int \mathrm{d}\mu_k \, \langle\alpha| \, v_t^k X_t^k v_t^{k\dagger} \, |\alpha\rangle \\
&= \int \mathrm{d}\mu_k \sum_\alpha \langle\alpha| \, v_t^k X_t^k v_t^{k\dagger} \, |\alpha\rangle \, . \qquad \text{(B.37)}
\end{aligned}$$

Note that the equality in Eq. (B.37) corresponds to the interchange of the Haar integral and the trace, which follows from the fact that both the trace and the Haar integral are linear functionals.

$$\begin{aligned}
\mathrm{Tr}\{[X_t^k]_{dd}\} &= \int \mathrm{d}\mu_k \, \mathrm{Tr}\left\{v_t^k X_t^k v_t^{k\dagger}\right\} \\
&= \int \mathrm{d}\mu_k \, \mathrm{Tr}\left\{X_t^k v_t^{k\dagger} v_t^k\right\} \qquad \text{(B.38)} \\
&= \int \mathrm{d}\mu_k \, \mathrm{Tr}\left\{X_t^k \mathbb{1}_{n_t^k}\right\} \qquad \text{(B.39)} \\
&= \mathrm{Tr}\left\{X_t^k \int \mathrm{d}\mu_k \, \mathbb{1}_{n_t^k}\right\} \qquad \text{(B.40)} \\
&= \mathrm{Tr}\left\{X_t^k\right\} . \qquad \text{(B.41)}
\end{aligned}$$

The equality in Eq.(B.38) follows from the cyclic property of the trace. We then utilize the unitarity of the operators v_t^k to obtain the equality in Eq.(B.39). Next, we commute the integral and the trace, as the Haar integral is evaluated only over the elements of $\mathcal{U}(n_t^k)$, which do not appear in Eq. (B.39). This commutation is permissible because the trace of X_t^k is treated as a constant. Finally, we use the fact that the Haar measure is normalized, i.e.:

$$\int \mathrm{d}\mu_k \, \mathbb{1}_{n_t^k} = \mathbb{1}_{n_t^k} .$$

On the other hand, we can evaluate the trace of the operator $[X_t^k]_{dd}$ using the equality Eq.(B.36), obtaining:

$$\mathrm{Tr}\{[X_t^k]_{dd}\} = \mathrm{Tr}\{C_t^k \mathbb{1}_{n_t^k}\} = C_t^k \, \mathrm{Tr}\{\mathbb{1}_{n_t^k}\} = C_t^k \dim\{\mathcal{H}_k\}. \qquad \text{(B.42)}$$

Thus, from Eq.(B.41) and Eq.(B.42), we can determine the constant C_t^k. Specifically,

$$\mathrm{Tr}\{[X_t^k]_{dd}\} = \mathrm{Tr}\left\{X_t^k\right\} = C_t^k \dim\{\mathcal{H}_k\} \implies C_t^k = \frac{\mathrm{Tr}\left\{X_t^k\right\}}{\dim\{\mathcal{H}_k\}}. \qquad \text{(B.43)}$$

Substituting C_t^k from Eq.(B.43) into Eq.(B.36), we obtain:

$$[X_t^k]_{dd} = \frac{\mathrm{Tr}\left\{X_t^k\right\}}{\dim\left\{\mathcal{H}_k\right\}}\mathbb{1}_{n_t^k},$$

which is the equality in Eq. (B.34). Therefore, the Lemma 4 is proved. ☐

With this result in hand, we can finally obtain the general result used in this work to evaluate Haar averages over the thermodynamic gauge group defined in Eq. (3.28). Given the significance of this result for our work, we state it as a Theorem below.

Theorem 11. *(Haar average) Let us consider the $\mathcal{G}$ group defined by:*

$$\mathcal{G} = \mathcal{U}(n_t^1) \times \mathcal{U}(n_t^2) \times \ldots \times \mathcal{U}(n_t^p) \tag{B.44}$$

which is a compact Lie group, similar to the structure to the gauge group defined in Eq. (3.28), which is associated to the Hilbert space $\mathcal{H}^d = \bigoplus_{k=1}^{p} \mathcal{H}_k$ where $p \leq d$ and $\dim\left\{\mathcal{H}_k\right\} = n_t^k$. Then, the Haar measure induced by the group (B.44) is given by:

$$d\mathcal{G} = \prod_{k=1}^{p} \mathrm{d}\mu_k, \quad \mathrm{d}\mu_k = \mathrm{d}\mu[\mathcal{U}(n_t^k)] \tag{B.45}$$

which $1 \leq k \leq p$. Therefore, the Haar average of any $d \times d$ matrix X over the $\mathcal{G}$ group is given by:

$$X_{dd} = \int d\mathcal{G}\mathcal{V}X\mathcal{V}^{\dagger} = \bigoplus_{k=1}^{p} \frac{\mathrm{Tr}\{X_{n_t^k}\}}{\dim\left\{\mathcal{H}_k\right\}}\mathbb{1}_{n_t^k}, \tag{B.46}$$

where $X_{n_t^k} = X\Pi_{n_t^k}$ with $\Pi_{n_t^k}$ being the projector of each subspace $\mathcal{H}_k$ and $\dim\left\{\mathcal{H}_k\right\} = n_t^k$.

Proof. Now, we going to obtain the relation (B.46). For this, we consider the

$$\begin{aligned}
X_{dd} &= \int d\mathcal{G}\; \mathcal{V}X\mathcal{V}^{\dagger} \\
&= \int d\mathcal{G} \bigoplus_{k=1}^{p} v_t^k \; X \bigoplus_{k=1}^{p} v_t^{k\dagger} \\
&= \sum_{k=1}^{p} \int d\mathcal{G}\, \mathcal{I}_k\left(v_t^k\right) X \mathcal{I}_k\left(v_t^{k\dagger}\right) \\
&= \sum_{k=1}^{p} \int \mathrm{d}\mu_k\; \mathcal{I}_k\left(v_t^k\right) \left(\sum_{\alpha} \left|\alpha\right\rangle\left\langle\alpha\right|\right) X \left(\sum_{\beta} \left|\beta\right\rangle\left\langle\beta\right|\right) \mathcal{I}_k\left(v_t^{k\dagger}\right) \\
&= \sum_{k=1}^{p} \int \mathrm{d}\mu_k\; \mathcal{I}_k\left(v_t^k\right) \left(\Pi_{n_t^k} X \Pi_{n_t^k}\right) \mathcal{I}_k\left(v_t^{k\dagger}\right)
\end{aligned}$$

where the projectors of all Hilbert space: $\sum_{\gamma} |\gamma\rangle\langle\gamma| = \mathbb{1}$ with $\gamma = \alpha, \beta$ effectively become the projectors onto the n_t^k subspace due to the other elements of the matrices $\mathcal{I}_k\left(v_t^k\right)$ and $\mathcal{I}_k\left(v_t^{k\dagger}\right)$ are zero outside this subspace.

Now, we going to define the following auxiliary matrix X_t^k as:

$$\mathcal{I}_k(X_t^k) = \Pi_{n_t^k} X \Pi_{n_t^k}, \tag{B.47}$$

where X_t^k is the restriction of X to the subspace defined by the projectors $\Pi_{n_t^k}$, resulting in an $n_t^k \times n_t^k$ matrix. Utilizing the preceding relation, the following development is obtained:

$$\begin{aligned}
X_{dd} &= \sum_{k=1}^{p} \int \mathrm{d}\mu_k \; \mathcal{I}_k\left(v_t^k\right) \mathcal{I}_k(X_t^k) \mathcal{I}_k\left(v_t^{k\dagger}\right) \\
&= \sum_{k=1}^{p} \int \mathrm{d}\mu_k \; \mathcal{I}_k\left(v_t^k X_t^k v_t^{k\dagger}\right) \\
&= \sum_{k=1}^{p} \mathcal{I}_k\left(\int d\mu_k v_t^k X_t^k v_t^{k\dagger}\right) \\
&= \bigoplus_{k=1}^{p} \frac{\mathrm{Tr}\{X_t^k\}}{\dim\{\mathcal{H}_k\}} \mathbb{1}_{n_t^k}
\end{aligned}$$

where the last equality follows from the Lemma (4). Finally, using the relation between X_t^k and X, we can obtain the following equality:

$$\mathrm{Tr}\left\{X_t^k\right\} = \mathrm{Tr}\{X \Pi_{n_t^k}\}. \tag{B.48}$$

In fact, to obtain Eq. (B.48), we evaluate the trace of $\mathcal{I}_k(X_t^k)$. First, applying the definition of immersion from Eq. (B.30), we find that for all k:

$$\mathrm{Tr}\left\{\mathcal{I}_k(X_t^k)\right\} = \begin{cases}
\mathrm{Tr}\left\{X_t^k \oplus \left(\bigoplus_{m=1}^{p-1} \mathbb{0}_{n_m}\right)\right\} = \mathrm{Tr}\left\{X_t^k\right\} \\[2ex]
\mathrm{Tr}\left\{\left(\bigoplus_{m=1}^{k-1} \mathbb{0}_{n_m}\right) \oplus X_t^k \oplus \left(\bigoplus_{m=k+1}^{p} \mathbb{0}_{n_m}\right)\right\} = \mathrm{Tr}\left\{X_t^k\right\} \\[2ex]
\mathrm{Tr}\left\{\left(\bigoplus_{m=1}^{p-1} \mathbb{0}_{n_m}\right) \oplus X_t^k\right\} = \mathrm{Tr}\left\{X_t^k\right\}
\end{cases}, \tag{B.49}$$

therefore, the trace is invariant under changes in k. On the other hand, using Eq. (B.47) and the cyclic property of the trace, we have:

$$\mathrm{Tr}\{\mathcal{I}_k(X_t^k)\} = \mathrm{Tr}\{\Pi_{n_t^k} X \Pi_{n_t^k}\} = \mathrm{Tr}\{X \Pi_{n_t^k}\}. \tag{B.50}$$

Combining Eq.(B.49) and Eq.(B.50), we arrive at the desired equality (B.48). Consequently, the Haar average of X can be expressed as:

$$X_{dd} = \bigoplus_{k=1}^{p} \frac{\mathrm{Tr}\{X_{n_t^k}\}}{n_t^k} \mathbb{1}_{n_t^k}.$$

Thus, the proof of the Theorem is complete. □

Corollary 3. *The Haar average of any matrix X is equal to the Haar average of the diagonal part of X.*

Proof. Trivial. □

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