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CICLO

XXIX

THERMODYNAMICS OF QUANTUM SYSTEMS DRIVEN FAR FROM EQUILIBRIUM

Settore Scientifico Disciplinare FIS/02

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To my Mother
and my Father

SINTESI

In questa Tesi sono riportati i diversi studi, condotti nei tre anni di dottorato, inerenti al campo della termodinamica quantistica dei sistemi fuori dall'equilibrio. Indubbiamente, il germe dal quale si è sviluppata gran parte dei lavori qui illustrati, è stato il paradigma dei teoremi di fluttuazione relativi al lavoro termodinamico compiuto in processi di non equilibrio. Nella fattispecie, nei nostri studi sono stati presi in esame dei processi di non equilibrio in sistemi quantistici chiusi, che vengono generati a causa del controllo esterno di alcuni parametri del sistema. Un'analisi di questi processi è stata condotta da un punto di vista teorico, sia considerando un generico processo di non equilibrio, per il quale la non adiabaticità dell'evoluzione è stata messa in relazione con le proprietà termodinamiche del processo; sia tramite alcuni studi in specifici sistemi fisici a molti corpi che presentano comportamenti critici. Inoltre, è stato affrontato il problema dell'estrazione del lavoro da un sistema quantistico avente il ruolo di batteria, prestando una particolare attenzione al ruolo svolto dalla coerenza e dalle correlazioni quantistiche in tali processi.

La Tesi è costituita da tre parti.

Nella **prima parte**, dopo un breve introduzione alla Tesi, nel Cap. 2 alcune nozioni, fondamentali ai fini della discussione, sono introdotte alla luce dell'uguaglianza di Jarzynski e del teorema di Tasaki-Crooks. Inoltre, il ruolo del lavoro termodinamico nel campo dell'informazione quantistica, è delineato attraverso alcune relazioni ricavate di recente, che sono state brevemente presentate.

Nella **seconda parte**, è presentato uno studio generale dei processi di nostro interesse. Nel Cap. 3, è discussa la termodinamica di non equilibrio, considerando due ipotetici processi di riferimento: una trasformazione reversibile isoterma e una trasformazione reversibile adiabatica. Quest'ultimo processo

permette di definire in modo naturale il cosiddetto "attrito quantistico interno", per il quale abbiamo ricavato una relazione di fluttuazione di Tasaki. Tale formalismo generale, è illustrato anche con l'aiuto di due esempi paradigmatici, che sono un oscillatore armonico e uno spin $1/2$. Nello stesso capitolo, è anche introdotta una misura entropica di non adiabaticità, che in circostanze particolari si identifica con l'attrito interno e che viene discussa da un punto di vista termodinamico, mostrando che essa può essere messa in relazione con il lavoro termodinamico compiuto nel processo. Il suo comportamento è stato altresì studiato nel caso in cui il processo tende ad essere adiabatico, trovando un'interessante relazione che coinvolge una misura della coerenza quantistica dello stato di un generico sistema, nota come entropia relativa di coerenza. Altre relazioni che coinvolgono tale misura di coerenza sono state riportate, seppure il ruolo della coerenza quantistica è ancora oggetto dei nostri studi. Nel Cap. 4, è condotto uno studio dei processi di estrazione di lavoro da "batterie quantistiche", con lo scopo di mettere in relazione le correlazioni quantistiche con il lavoro estratto. Qui, viene proposta e studiata in termini generali una nuova procedura di estrazione di lavoro, che fa uso delle correlazioni condivise tra il sistema e un ulteriore sistema ausiliario. In linea di principio, il processo di estrazione può essere ottimizzato facendo uso dell'informazione sullo stato del sistema, acquisita per mezzo di misure locali compiute sul sistema ausiliario. L'esistenza di correlazioni quantistiche tra i due sottosistemi può essere investigata, guardando il cosiddetto guadagno "demoniaco" sul lavoro. Tale procedura è stata discussa anche prendendo in considerazione un sistema di due qubit.

La **terza parte** contiene la caratterizzazione di processi di non equilibrio in specifici sistemi quantistici. Nel Cap. 5 è considerato il modello quantistico di Ising in campo trasverso, il quale viene bruscamente allontanato dall'equilibrio per mezzo di una perturbazione localizzata sul bordo del sistema. Il sistema è studiato grazie ad una rappresentazione fermionica, e la termodinamica di non equilibrio è stata caratterizzata in termini del lavoro compiuto in questo processo, che è stato messo in relazione con la transizione di fase quantistica del sistema. Tale modello è legato alla cosiddetta catena di Kitaev, nella quale è presente un modo di Majorana ad energia nulla. Per capire a fondo il ruolo giocato dal modo di Majorana nella dinamica di fuori equilibrio, è stata studiata la propagazione di una perturbazione locale lungo la catena, valutandola tramite la magnetizzazione trasversa, la quale presenta forti oscillazioni proprio a causa del coinvolgimento di tale modo ad energia nulla. Nel Cap. 6 è considerato il modello di Dicke. Questo è un altro modello critico, che descrive l'accoppiamento di un numero elevato di atomi con un modo normale di un risonatore elettromagnetico. In tale sistema, è stato considerato il processo di non equilibrio prodotto da una forzante applicata agli atomi. Dal punto di vista tecnico, la dinamica è stata descritta in termini dei campi medi e delle fluttuazioni quantistiche attorno ad essi. In particolare, le circostanze sotto cui le fluttuazioni diventano illimitate nel tempo sono state discusse in generale, e caratterizzate nel caso di una forzante periodica facendo uso del teorema di Floquet. In particolare, si è visto che è possibile provocare una produzione di fotoni dal vuoto a causa dell'amplificazione parametrica delle fluttuazioni. Questo meccanismo, che simula l'effetto di Casimir dinamico, è stato messo in relazione con la termodinamica di non equilibrio, attraverso una caratterizzazione del lavoro termodinamico compiuto dalla forzante e dell'attrito interno quantistico provocato a causa della non adiabaticità del processo.

ABSTRACT

In this Thesis, I would present the work done during my Ph.D. course, in the last three years. These studies have been focused on non equilibrium processes in quantum systems, and have led to several different interesting results, which are undoubtedly rooted in the field of the quantum thermodynamics.

We have performed a general theoretical analysis, allowing to characterize the thermodynamic irreversibility of this kind of processes $[A]$.This is content of part of the Thesis, consisting of Chap. 3. Then, we considered some particular physical systems, among which quantum spin chains $[B, C]$, and a Dicke model $[D]$. A new kind of work extraction protocol has been also proposed $[E]$, in which the presence of quantum correlations plays a crucial role.

CONTENTS

Part I.

Introduction and Background Materials

1 INTRODUCTION

Out of equilibrium processes, in which a physical system evolves in time starting from or being brought to a non equilibrium configuration, are ubiquitous in nature. Examples are a fast compression of a gas could produce internal relative motions, with a subsequent irreversible increase of its internal energy, or intrinsically irreversible processes, like the mixing of two gases of different species, or the spontaneous heat transfer from a hot body to a cold one, which could drive the system through a sequence of non equilibrium states.

In a physical system, an out of equilibrium process could be generated by changing its external conditions fast enough in time.

In principle, a simple description of such phenomena in terms of few "thermodynamic" quantities is often possible, by referring them to ideal quasi-static processes.

However, as the real process is too far from the ideal one, such a description unavoidably falls down. Anyway, under certain conditions, it is possible to constrain the thermodynamic quantities to some emergent rules. These rules need to emerge from the underlying fundamental principles describing the microscopic costituents of matter. A common example is the second principle of thermodynamics, but several more restrictive constraints could follow, that are usually referred to as *fluctuation theorems*. These theorems, introduced and object of discussion in Chap. 2, are usually expressed in terms of statistical relations, where usually a non equilibrium fluctuating quantity is related to the equilibrium properties of an ideal reference trasformation.

In the last few years, the technological progress has allowed exceptional experiments in which the quantumness plays a crucial role [1, 2]. They have opened the way to infer about several interesting theoretical problems [3, 4], among which the thermalization problem in closed systems [5], and the production of defects due to the spontaneous breaking of a symmetry [6, 7].

This has contributed to keep a keen interest in the developing of the paradigm of the fluctuation theorems and in the study of thermodynamics in the quantum realm. Doubtless, a fundamental quantity in this context is the energy that the system exchanges with its environment during transformation or non equilibrium process. In the last three years, our focus has been directed towards those processes in which a high degree of isolation is reached, so that the system can be manipulated by keeping a unitary time evolution. In these cases, the process is generated by some driving agent, and some of *work* is done on the system.

Being performed on microscopic systems, this work is affected by random fluctuations, which are constrained by statistical relations, as illustred in Chap. 2 and in Chap. 3.

In this scenario, although the process obtained is typically irreversible, the ideal reversible transformations keep playing a reference role in the description. In Chap. 3, two reversible transformations, an isothermal and an adiabatic transformation, are examined, allowing to characterize the amount of "irreversible work" produced $[A]$.

There, we also show how the distance from the reversible transformation is unavoidably linked to the quantum coherence generated in the process $[F]$.

We also analysed the work *extraction* processes from a storing center of energy which are discussed in Chap. 4. The work extracted can have a purely quantum contribution, due solely to quantum coherence and having no classical counterpart $[F]$.

Indeed, the existence of correlations between the storing center, and an auxiliary system subject to measurement, can enhance the work extracted if a local feedback control is used. Furthermore, the gain in work achieved in this way is intimately related to the quantumness of such correlations $[E]$. As a result, this feedback protocol can be used to investigate about the nature of the correlations between the parts of a quantum system.

The work should be related also to other non equilibrium properties, depending on the particular system under consideration.

We have considered mostly spin 1/2 systems. In particular, a system with Ising interactions is the subject of Chap. 5. Such a system can be brought far from the equilibrium by a "quench" in the applied magnetic field. In particular, we considered a quench that is localized at its boundary. The work perfomed by the driving agent that modifies the field is studied in some limiting circumstances, showing a behavior typical of the critical systems. The propagation along the chain of the disturbance generated after the quench, is also well characterized in terms of the magnetization of the system.

Another spin system, in which the interactions are mediated by a common bosonic field, is considered in Chap. 6. Specifically, we study the dynamics of a driven system of atoms, collectively interacting with a quantum electromagnetic mode in an optical cavity (Dicke model). In such a system, under a periodic perturbation, photons could be generated from the vacuum state because of a parametric amplification of the quantum fluctuations. Also this process, mimicking the dynamical Casimir effect, is well characterized in terms of the work done.

Summarizing, this Thesis is essentially structured in three main parts, and some appendices, added in order to lighten the discussion in the main parts.

The **first part** contains an introduction to the dissertation, and some useful background materials. Substantially, we briefly introduce the framework of the fluctuation theorems in Chap. 2, mainly with the aim of outlining how our results are placed in the present-day research scenario. There, the thermodynamic work is discussed as a statistical quantity, and both the Jarzynski relation and the Crooks theorem are discussed in general. Some recent relations between the work and the field of the quantum information theory are also considered.

In the **second part**, we present a general study of thermodynamic processes of interest. In Chap. 3, we focus on the non equilibrium thermodynamics in driven closed quantum systems, mainly presenting the results reported in $[A]$. There, the real out of equilibrium process is compared to two different hypothetical transformations: a reversible isothermal transformation and a reversible adiabatic one. Then, the study is carried on by taking into account the irreversible amount of work produced in the process, that should be quantified in terms of either the inner friction $\left\langle w_{fric}\right\rangle$, or the irreversible work $\langle w_{irr}\rangle$, depending on the reversible transformation used as a reference. Furthermore, we discuss also how the quantum non adiabaticity of the time evolution affects the thermodynamic work done. There, we derive some interesting relations involving thermodynamic quantities and a measure of quantum coherence. In Chap. 4 we propose a new link between the field of thermodynamics and of quantum information theory. We show how the thermodynamics can be related to the correlations in a bipartite state. Specifically, the presence of quantum correlations could be inferred by looking the performance of a suitable work extraction protocol [E].

In the **third part**, we present a characterization of the non equilibrium thermodynamics in two different many-body systems. In Chap. 5, we consider a quantum Ising spin chain in a transverse field, that is suddenly brought out of equilibrium by a disturbance localized on its boundary. The study of this process should be relevant, because of the relation between such system and the Kitaev chain, which allows for the possibility to have two so-called Majorana zero modes, localized at the edges of the chain. The thermodynamics of the process is characterized in terms of the work done, its moments and the amount of irreversible work produced. We demonstrate that these quantities display a signature of the critical behavior of the system at the quantum phase transition point.

Furthermore, the propagation of the disturbance in the transverse magnetization of the chain is analysed, underlining the role played by the Majorana zero mode, that could be involved in the dynamics [C].

In Chap. 6 we consider another physical system, described by a Dicke model. The out of equilibrium process is generated by considering a general parametric driving, and the dynamics of the system is studied by using a general framework, that would give an exact description for an infinite number of atoms [D]. The quantum fluctuations could undergo an unbounded time evolution for such a system in the super-radiant phase, and this effect is carefully characterized in the particular case of a periodic driving. A mechanism similar to the dynamical Casimir effect can arise in this case, permitting the generation of photons from the quantum vacuum state. This effect is linked to the non equilibrium thermodynamics of the process, by studying the work done and the inner friction produced.

2 FLUCTUATION THEOREMS

In this Chapter, we give a quick overview of the paradigm of the fluctuation theorems in the context of out of equilibrium processes.

Most of the arguments discussed here are reconsidered again in Chap. 3, in the case of a closed quantum system.

We briefly discuss the concept of the thermodynamic work in the quantum regime, and the fluctuation theorem satisfied by its distribution in Sec. 2.1. Mostly, we focus on the Jarzynski equality [8], that allows us to introduce some fundamental concepts, like the irreversible work, which is then used many times in subsequent Chapters.

In the Sec. 2.2 we give a succinct presentation of some recently derived relations between this paradigm and the field of the information theory. Some works that outline the role of the quantum correlations in a quantum thermodynamic process are also illustrated. This is done with the aim of placing the results of Chap. 4 in the present-day research context.

2.1 WORK FLUCTUATION THEOREMS

The description of a physical system in terms of the fundamental microscopic laws usually tends to be useless with the increase of the degrees of freedom of the system. Luckily, the microscopic constituents of a physical system typically are in a permanent state of agitation, so that a statistical study can be carried on; then the physical quantities of interest will be thought as statistical quantities, affected by random fluctuations [9].

In several cases these fluctuations are weak, and a description in terms of the mean values is enough.

Here we focus on the out equilibrium processes, in which a physical system is driven far of equilibrium by some changes in its external condition or potential. In this context too, the influence of the fluctuations could play a dominant role in the statistical description.

Usually a parameter λ of the system, referred to as *work parameter*, is varied in a certain time interval $[0, \tau]$, and an amount of work is performed on the system because of that.

Technically, we consider a process to be defined as the protocol in which the parameter λ is changed from the initial value λ_i at the time $t = 0$, to the final value λ_f at the time $t = \tau$, by following a given functional relation

$$\lambda : t \in [0, \tau] \mapsto \lambda(t) \tag{1}$$

The work turns out to be described by a stochastic quantity w characterized by a probability distribution $p(w)$, so that its mean value is given by [10] $\langle w \rangle = \int wp(w)dw$.

For instance, in a quasistatic isothermal trasformation, if the system stays in equilibrium with a heat bath at the temperature T at any time of the process, the work is the difference of the Helmholtz free energy, ΔF, evaluated at the final and the initial equilibrium states, that is $\Delta F = F[\lambda_f, T] - F[\lambda_i, T]$, where with $F[\lambda, T]$ we indicate the Helmholtz free energy of the equilibrium state $[\lambda, T]$.

In finite time processes, instead as the fluctuations of the work become strong, higher moments of the work distribution are needed to accurately characterize the work. They can be calculated from the characteristic function χ, where

$$\chi(u) = \int e^{iuw} p(w)dw \tag{2}$$

as $\langle w^n \rangle = (-i)^n \chi^{(n)}(0)$.

Jarzynski in [8] found that, when the quantum effects can be neglected, the work fluctuations are constrained by the relation

$$\left\langle e^{-\beta w} \right\rangle = e^{-\beta \Delta F} \tag{3}$$

provided that initially the system is described by a canonical ensemble at the temperature $T = (k_B\beta)^{-1}$, and that, during the process, the system can be considered thermodynamically isolated, or weakly interacting with an heat bath at the same temperature T. In the last case, the amount of energy $\langle w\rangle - \Delta F$, which can be associated with the increase of entropy during an irreversible process, is always non negative, since from Eq. (3) it follows that $\langle w\rangle \geq \Delta F$ [8].

If the fluctuations can be neglected, the work for the typical trajectories in the phase space, would be approximated by the average value $\langle w\rangle$, and so $\langle w\rangle \approx \Delta F$, by using Eq. (3).

Furthermore, from Eq. (3), the probability $P(w < \Delta F - \zeta)$ to observe a value of work smaller than $\Delta F - \zeta$, turns out to be bounded as [11]

$$P(w < \Delta F - \zeta) < e^{-\beta\zeta} \tag{4}$$

where ζ is an arbitrary positive value with the units of energy.

Then, the left tail of the distribution probability $p(w)$ becomes exponentially suppressed in the thermodynamically forbidden region $w < \Delta F$, in agreement with the second law of thermodynamics.

The free energy ΔF can be obtained as a sum of the cumulants ω_n of the work distribution function [1], because Eq. (3) implies the expansion [11]

$$\Delta F = \sum_{n=1}^{\infty} (-\beta)^{n-1} \frac{\omega_n}{n!} \tag{5}$$

The Eq. (5) allows to compute the difference ΔF in terms of the cumulants of the work, and, in the linear response (or Gaussian) regime, the fluctuation dissipation theorem

$$\langle w\rangle - \Delta F \simeq \frac{\beta}{2}\left(\langle w^2\rangle - \langle w\rangle^2\right) \tag{6}$$

follows as a limiting case of Eq. (5).

A deeper characterization of the work performed can be done by comparing this “forward” process with the corresponding “backward” one [10].

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1 The cumulant ω_n can be calculated from the generating function $g(u) = \ln(\chi(u))$, as $\omega_n = (-i)^n g^{(n)}(0)$.

In principle, the backward process is obtained by time reversing the trajectories in the phase space of the system. However, if the system is time reversal symmetric, this process could be achieved as the parameter λ retraces its history in time.

The fluctuations of the work in these two protocols are not statistically independent, as it is highlighted by the Crooks fluctuation theorem

$$p(w)e^{-\beta(w-\Delta F)} = \overline{p}(-w) \tag{7}$$

where $\overline{p}(w)$ is the probability distribution of the work done when the system is driven in a time-reversed manner [12].

The fluctuation theorem in Eq. (7) is more general than the relation in Eq. (3). Indeed, Eq. (3) can be derived by integrating both sides of Eq. (7) with respect to w.

By looking at Eq. (7), it is clear that the trajectories in phase space for which the work is larger than ΔF, tend to be "exponentially" preferred than their time reversed trajectories, and so the probability of a violation of the second principle of thermodynamics is exponentially small.

The distance of the work distribution function $p(w)$ from its time reversed counterpart $\overline{p}(-w)$ can be characterized by the relative entropy (also known as Kullback-Leibler divergence)

$$D_{KL}(p(w)||\overline{p}(-w)) = \int p(w)\ln(p(w)/\overline{p}(-w))dw\,. \tag{8}$$

By using Eq. (7), it is found that [13]

$$D_{KL}(p(w)||\overline{p}(-w)) = \beta(\langle w\rangle - \Delta F)$$

This helps to understand how the thermodynamic arrow of time arises from an underlying time reversible dynamics, which is an unresolved problem in physics [14].

In this Thesis, we will refer to the quantity $\langle w\rangle - \Delta F$ as irreversible work, and we indicate it with $\langle w_{irr}\rangle$.

It is not obvious how to formulate the same relationships, if the quantum effects cannot be neglected. Essentially because, differently from the classical regime, the work cannot be measured by continuously monitoring the system, without a drastic change in the dynamics due to the wave function collapse.

There are several approaches to the formalism of the fluctuation theorems for quantum systems. For instance, they can formulated thanks a two measurements protocol [15, 10], that essentially finds its bases in the relations discovered by Tasaki in [16], or by using a quantum trajectory formalism [17, 18]. In particular, the Jarzynski equality in Eq. (3) discussed in this Chapter, can be explicitly derived also if the quantum nature of the system is taken into account [19].

Fluctuation relations have been formulated also for the exchange of heat from a hot to a cold bath [20, 21, 22], and for a general heat engine [23].

Several investigations have been done, among which, experiments have been reported where work is measured by using a two projection method [24], an interferometric method [25], and a quantum jump method [26].

The characterization of the thermodynamic work in closed quantum systems is discussed in detail in Chap. 3, where the work is put in relation with other thermodynamics quantities, like the irreversible work and the inner friction, and with the non adiabaticity of the out of equilibrium process and the quantum coherence generated during the protocol.

2.2 THERMODYNAMICS AND INFORMATION THEORY

Doubtless, in understanding the relation between the information theory and the field of the thermodynamics [27, 28], the experiment proposed by Szilard [29] plays a key role. It shows how a positive amount of work can be performed by using only one heat bath, thanks to a Maxwell's demon that plays the role of a feedback controller [30, 31].

In this context, typically, the second law of thermodynamics is discussed by taking into account the erasure process of the memory used by the demon [32, 33, 34, 35, 27]. Recently, the thermodynamics of a Landauer erasure process has been studied in [36] by using a fluctuation relation, and a lower bound for the heat exchange has been found.

For an isothermal process, the second law reads $\langle w \rangle \geq \Delta F$, and by using a feedback control, the work done on the system can be lowered thanks to the information acquired in the measurement process, as shown by Sagawa and Ueda in [37].

Specifically, if in order to perform the feedback control, the information on the state of the system is acquired by using a positive-operator valued measure [38], the work done will be [31]

$$\langle w \rangle \geq \Delta F - k_B T I_{QC} \tag{9}$$

where the quantity I_{QC} is the so called Quantum-Classical mutual information [31]. If the measurement process is described by the positive value operators $\{\hat{E}_k = \hat{M}_k^\dagger \hat{M}_k\}_k$, and the state of the system at the instant of measurement is $\hat{\rho}$, so that it collapses onto $\hat{\rho}_k = \hat{M}_k \hat{\rho} \hat{M}_k^\dagger / p_k$ with the propability $p_k = \mathrm{Tr}\left\{\hat{\rho}\hat{E}_k\right\}$, then the Quantum-Classical mutual information can be expressed as $I_{QC} = S(\hat{\rho}) - \sum_k p_k S(\hat{\rho}_k)$, where $S(\hat{\rho})$ is the Von Neumann entropy

$$S(\hat{\rho}) = -\mathrm{Tr}\left\{\hat{\rho} \ln \hat{\rho}\right\} \tag{10}$$

Fluctuation theorems are discussed for generalized thermodynamic observables when the dynamics is described by a completely positive trace preserving map, with and without feedback control in [39].

The equality in Eq. (9) can also be obtained, as shown by Jacobs in [40], and so by using a cyclic transformation, it is possible to extract the amount of work $k_B T I_{QC}$ from a heat bath at temperature T.

The role played by the non local nature of the quantum correlations [41, 42] in the work extraction from a thermal bath has received a certain attention [43, 44, 28]. In particular, in [43] it is shown that the amount of work extracted by considering a bipartite state shared by two parties is less than the amount of work extractable when one part is in possession of the entire state. The resulting work deficit is discussed as a measure of the quantum correlations in the global state.

The quantum correlations, characterized by the quantum discord [45, 46, 42], can be also related to the thermodynamics of a work extraction protocol, as shown in Chap. 4.

2.3 SUMMARY AND CONCLUSIONS

In this Chapter, we have illustrated the paradigm of the fluctuation theorems, by introducing some fundamental relations, such as the Jarzynski equality, and the Crooks theorem. The importance of these relations has been clarified, by considering the different physical implications arising from them. We have also briefly described how these relations can be related to information theory, and to quantum correlations.

Part II.

General Theoretical Analysis

3 QUANTUM THERMODYNAMICS PROCESSES

In this Chapter we discuss the thermodynamics of out of equilibrium processes in closed quantum systems.

In particular, Sec. 3.1 is about the concept of thermodynamic work in closed quantum systems. Specifically, it is shown how its statistics can be obtained in a two measurement protocol.

In Sec. 3.2 we focus on the case in which the system is prepared in a thermal Gibbs state. Here, a key quantity, the so called inner friction, is introduced, discussed and compared with the irreversible work [A]. Both the two quantities are related with the heat exchange with a heat bath in specific thermalization processes. The inner friction is also related to the entropy produced, and can be recast in terms of a quantum relative entropy. This framework is applied to two paradigmatic processes: a harmonic oscillator with a parametrically driven frequency in Sec. 3.2.1, and a Landau-Zener process in Sec. 3.2.2.

In Sec. 3.3, we focus on the use of the ideal adiabatic evolution as a reference transformation for the actual out of equilibrium process. Then, we show how the work done depends on the non adiabaticity of the process.

The role played by the coherence generated during the process is also studied and investigated in terms of some thermodynamic quantities.

Some of the concepts introduced here will be useful for the characterization of driving processes in two specific physical systems: the quantum Ising model in Chap. 5 and the Dicke model in Chap. 6.

In the following sections, some results are stated without a full derivation, which has rather been included in the technical appendices at the end of the Chapter.

3.1 WORK IN CLOSED QUANTUM SYSTEMS

A system, whose time evolution is described by the time-dependent Schrödinger equation, is referred to as closed (or isolated) quantum system.

In a real physical system, this kind of evolution can be achieved for times shorter than the dissipation and decoherence times [47].

Then, if a quantum system can be considered as closed, its average energy can vary only if some parameter of the Hamiltonian is changed in time. Since there is no energy dissipation during the process, an increase in the average energy of the system can be interpreted as work done $\langle w \rangle$ on the system by manipulating that parameter.

As in the classical case of the previous Chapter, we consider the case in which a parameter λ of the Hamiltonian is controlled in the time interval $[0, \tau]$, which changes from λ_i into λ_f by following the protocol in Eq. (1). The time evolution of the system's state is described by the unitary operator $\hat{U}_{t,0}[\lambda]$ generated by the time dependent Hamiltonian $\hat{H}(\lambda(t))$, and obtained as the solution of the Schrödinger equation [1]

$$i\frac{\partial}{\partial t}\hat{U}_{t,0}[\lambda] = \hat{H}(\lambda(t))\hat{U}_{t,0}[\lambda] \tag{11}$$

with the initial condition $\hat{U}_{0,0}[\lambda] = \mathbb{1}$.

If we indicate with $\hat{\rho}_i$ the initial density matrix of the system, the work done can be defined as

$$W = \mathrm{Tr}\left\{\hat{H}_f\hat{\rho}_\tau\right\} - \mathrm{Tr}\left\{\hat{H}_i\hat{\rho}_i\right\} \tag{12}$$

where the final state $\hat{\rho}_\tau$ is $\hat{\rho}_\tau = \hat{U}_{\tau,0}[\lambda]\hat{\rho}_i\hat{U}^\dagger_{\tau,0}[\lambda]$, and we have defined $\hat{H}_i = \hat{H}(\lambda_i)$ and $\hat{H}_f = \hat{H}(\lambda_f)$.

Unlike a state function, the work characterizes a process, rather than a state of the system, and in general it cannot be represented by a Hermitian operator whose eigenvalues can be determined in a single projective measurement.

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1 In this Thesis the energy units are always choosed so that $\hbar = 1$.

A way to define the work w as a random variable with probability distribution $p(w)$ is that of performing projective energy measurements at the beginning and at the end of the process [48, 10] and obtaining w as the difference.

In this framework, a first projective measurement of the energy is done at the initial time $t = 0$. Then, the parameter λ is varied in the time interval $(0, \tau)$, and afterwards a second projective measurement of the energy is performed at the time $t = \tau$.

If we indicate with $\left|\epsilon_n^{(i,f)}\right\rangle$ the eigen-state of $H_{i,f}$ with eigenvalue $\epsilon_n^{(i,f)}$, the probability distribution of work can be defined as

$$p(w) = \sum_n \sum_m P_m^{(i)} P_{m\to n}(\tau) \delta\left(w - \epsilon_n^{(f)} + \epsilon_m^{(i)}\right) \tag{13}$$

where $P_n^{(i)}$ is the initial population of the state $\left|\epsilon_n^{(i)}\right\rangle$, and $P_{m\to n}(\tau)$ is the transition probability $P_{m\to n}(\tau) = \left|\left\langle \epsilon_n^{(f)}\right| \hat{U}_{\tau,0}[\lambda] \left|\epsilon_m^{(i)}\right\rangle\right|^2$.

The stochasticity of the work is due to the (classical) fluctuations coming from the initial state $\hat{\rho}_i$, that have a thermal nature if the state is prepared by using a heat bath, and also to the quantum fluctuations if the time evolution is non adiabatic, so that each post-measurement time evolved state does not coincide with a unique energy eigenstate.

The statistics of the work done is fully encoded in the characteristic function $\chi(u)$, that has the form of a two-time quantum correlation function [48]

$$\chi(u) = \left\langle \hat{U}^\dagger_{\tau,0}[\lambda] e^{iu\hat{H}_f} \hat{U}_{\tau,0}[\lambda] e^{-iu\hat{H}_i} \right\rangle_i \tag{14}$$

where the average is calculated as $\langle \cdots \rangle_i = \mathrm{Tr}\left\{\cdots \hat{\Delta}^{(i)}(\hat{\rho}_i)\right\}$, where $\hat{\Delta}^{(i)}$ is the dephasing operator defined by

$$\hat{\Delta}^{(i)}(\hat{\rho}_i) = \sum_m \hat{\Pi}_m^{(i)} \hat{\rho}_i \hat{\Pi}_m^{(i)}, \tag{15}$$

with $\hat{\Pi}^{(i)} = \left|\epsilon_m^{(i)}\right\rangle \left\langle \epsilon_m^{(i)}\right|$. By using the time ordering operator $\hat{T}_>$, the characteristic function can be expressed as

$$\chi(u) = \left\langle \hat{T}_> e^{iu\int_0^\tau \partial_t \hat{H}^{(H)}(\lambda(t))dt} \right\rangle_i \tag{16}$$

where $\hat{H}^{(H)}(\lambda(t)) = \hat{U}^\dagger_{t,0}[\lambda]\hat{H}(\lambda(t))\hat{U}_{t,0}[\lambda]$. The probability distribution $p(w)$ in Eq. (13) is related to the characteristic function $\chi(u)$ in Eq. (14) by a Fourier transform.

The statistics of the work can be measured also by performing a generalized quantum measurement at a single time, instead of two projective measurements, as proposed in [49].

The average value $\langle w\rangle$ obtained from $\chi(w)$ reads

$$\langle w\rangle = \sum_n \left(P_n(\tau)\epsilon_n^{(f)} - P_n^{(i)}\epsilon_n^{(i)}\right) \tag{17}$$

where $P_n(\tau)$ is given by $P_n(\tau) = \sum_m P_m^{(i)} P_{m\to n}(\tau)$.

The average work $\langle w\rangle$ in Eq. (17) can be different from the work in Eq. (12), if the initial state $\hat{\rho}_i$ does not commute with the initial Hamiltonian $\hat{H}_i$. Essentially, the contributions to the work due to the coherences of $\hat{\rho}_i$ are lost in performing the projective measurements of the energy at the time $t = 0$.

From Eq. (16), the moments of the work distribution can be written as [50]

$$\langle w^n\rangle = \sum_{k=0}^{n} (-1)^k \frac{n!}{k!(n-k)!} \left\langle \hat{H}_f^{(H)n-k} \hat{H}_i^k \right\rangle_i \tag{18}$$

where $\hat{H}_f^{(H)} = \hat{H}^{(H)}(\lambda(\tau)) = \hat{U}^\dagger_{\tau,0}[\lambda]\hat{H}_f\hat{U}_{\tau,0}[\lambda]$. The first moment is equal to the average work given in Eq. (17), and the next two moments are

$$\begin{aligned} \langle w^2\rangle &= \left\langle (\hat{H}_f^{(H)} - \hat{H}_i)^2 \right\rangle_i \\ \langle w^3\rangle &= \left\langle (\hat{H}_f^{(H)} - \hat{H}_i)^3 \right\rangle_i + \left\langle [\hat{H}_f^{(H)}, \hat{H}_i](\hat{H}_f^{(H)} - \hat{H}_i) \right\rangle_i \end{aligned} \tag{19}$$

from which we see that the non commutativity of the energy at different times starts to manifest it sell from the third moment of the work.

The rate of change of the work parameter λ plays a crucial role, and we can distinguish the two limiting cases in which τ is very small (sudden change) and very large (adiabatic change).

For a sudden change, the time evolution operator can be approximated with the identity, and the characteristic function reads

$$\chi(u) = \left\langle e^{iu\hat{H}_f} e^{-iu\hat{H}_i} \right\rangle_i \tag{20}$$

In this particular case, when the initial state is an eigen-state of $\hat{H}_i$, the modulus square of $\chi(u)$ can be formally related to the so-called Loschmidt echo [51], which quantifies the revival occurring when an "imperfect" time-reversal procedure is applied to a complex quantum system.

3.2 IRREVERSIBLE WORK AND INNER FRICTION

In order to characterize the process in terms of the fluctuation relations discussed in Chap. 2, we consider the case in which the initial state is a thermal Gibbs state $\hat{\rho}_i = \hat{\rho}_G[\lambda_i, T_i]$, where

$$\hat{\rho}_G[\lambda, T] = \frac{e^{-\beta \hat{H}(\lambda)}}{Z[\lambda, T]} \tag{21}$$

Here $Z[\lambda, T] = \mathrm{Tr}\left\{e^{-\beta \hat{H}(\lambda)}\right\}$ is the canonical partition function, and the Helmholtz free energy $F[\lambda, T]$ can be calculated as $F[\lambda, T] = -\ln(Z[\lambda, T])/\beta$ [2].

Then, the initial populations are given by $P_n^{(i)} = e^{-\beta_i \epsilon_n^{(i)}}/Z[\lambda_i, T_i]$, and indeed the Jarzynski relation in Eq. (3) holds [48], allowing us to define the irreversible work $\langle w_{irr} \rangle = \langle w \rangle - \Delta F$ as a non negative quantity.

Typically, the reversible transformations, in which the system is driven from an equilibrium configuration to another one very slowly, can be used as a reference in order to characterize the performances of real processes.

However, if the system is pushed faster than the thermalization time, the transformation is irreversible, and can lead outside the manifold of equilibrium states.

2 The thermodynamic entropy can be calculated as $S[\lambda, T] = k_B S(\hat{\rho}_G[\lambda, T])$, where $S(\hat{\rho})$ is the Von Neumann entropy defined in Eq. (10), and the relation $F[\lambda, T] = TS[\lambda, T] - \mathcal{U}[\lambda, T]$ is fulfilled, where $\mathcal{U}[\lambda, T]$ is the internal energy.

In this context, the irreversible work $\langle w_{irr}\rangle$, is a measure of how far is the out of equilibrium process from a hypothetical isothermal reversible transformation, which would lead the system to the equilibrium state $\hat{\rho}_B = \hat{\rho}_G[\lambda_f, T_B = T_i]$.

This is made evident by expressing the irreversible work as [52]

$$\langle w_{irr}\rangle = \beta_B^{-1} D(\hat{\rho}_\tau || \hat{\rho}_B) \tag{22}$$

where

$$D(\hat{\rho}_1||\hat{\rho}_2) = \mathrm{Tr}\left\{\hat{\rho}_1\left(\ln\hat{\rho}_1 - \ln\hat{\rho}_2\right)\right\} \tag{23}$$

is the quantum relative entropy (or quantum Kullback-Leibler divergence) of $\hat{\rho}_1$ with respect to $\hat{\rho}_2$.

In an isothermal process, the state $\hat{\rho}_\tau$ usually does not lay on the manifold of equilibrium states because of a lag of the evolved state behind the instantaneous Gibbs state, as τ is too short compared with the relaxation times [47].

This is our case, since the system is assumed to be closed during the process. Anyway, starting from $\hat{\rho}_\tau$, the system can be lead to the equilibrium state $\hat{\rho}_B$ by a thermalization process (i.e. by keeping it in contact with a heat bath at the temperature T_i), in which the system takes the energy $\langle Q^{th}_{\tau\to B}\rangle = \mathrm{Tr}\left\{\hat{H}_f(\hat{\rho}_B - \hat{\rho}_\tau)\right\}$, and the irreversible work can be expressed as

$$\langle w_{irr}\rangle = T_i(S_B - S_i) - \langle Q^{th}_{\tau\to B}\rangle \tag{24}$$

where S_B and S_i are the thermodynamic entropies of the equilibrium states $\hat{\rho}_B$ and $\hat{\rho}_i$ respectively, and so $T_i(S_B - S_i)$ is the heat exchanged in the ideal reversible isothermal transformation.

If the coherence times are sufficiently long, and if the hypothesis for which the adiabatic theorem holds are satisfied [53], then it is also possible to achieve an adiabatic time evolution, that leads the system to the final state

$$\hat{\rho}_A = \hat{U}_A\hat{\rho}_i\hat{U}_A^\dagger = \sum_n P_n^{(A)}\hat{\Pi}_n^{(f)} \tag{25}$$

with $P_n^{(A)} = P_n^{(i)}$ and $\hat{\Pi}_n^{(f)} = \left|\epsilon_n^{(f)}\right\rangle\left\langle\epsilon_n^{(f)}\right|$.

It is then natural to introduce the so called inner friction $\langle w_{fric}\rangle$ defined by

$$\langle w_{fric} \rangle = \langle w \rangle - \langle w_{i \to A} \rangle \tag{26}$$

where $\langle w_{i \to A} \rangle$ is the work done on the system in the ideal adiabatic process. These adiabatic transformations enter the Carnot and the Otto cycles and have been, therefore, largely studied and discussed so far, in particular the role of the inner friction in an Otto cycle has been recently discussed in [54].

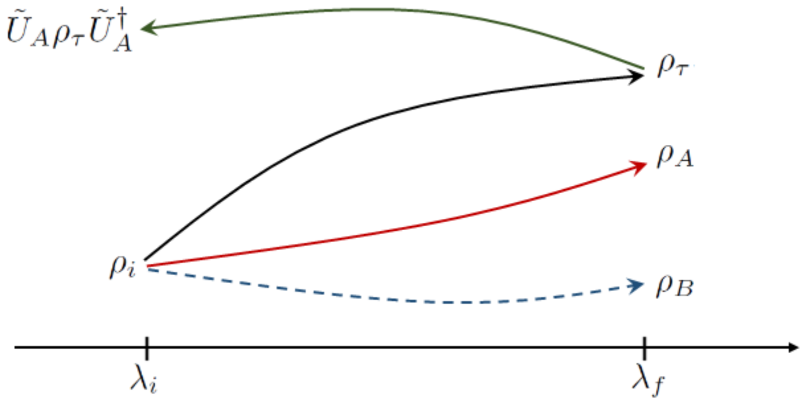

Figure 3.2.1.: The diagram summarizes the processes in the main text. The isothermal reversible transformation is represented by the blue dashed line, while the unitary processes are represented by solid lines. In particular the real process $U_{\tau,0}[\lambda]$ is indicated with the black line, and the two ideal adiabatic processes, described by U_A and $\tilde{U}_A$, by the red and the green line, respectively.

In principle, the adiabatic process is realized by changing the parameter λ in a sufficiently slow way, so that the transitions between instantaneous eigenstates of the energy are inhibited. Then at any moment during the transformation the system is in a stationary state, that does not have necessarily the form of a Gibbs state given in Eq. (21).

An adiabatic process for which the state of the system stays in the manifold of thermal Gibbs states, and the state $\hat{\rho}_A$ is $\hat{\rho}_A = \hat{\rho}_G[\lambda_f, T_A]$ for a certain temperature T_A, is possible if and only if there exists a T_A such that the condition $T_i(\epsilon_n^{(f)} - \epsilon_m^{(f)}) = T_A(\epsilon_n^{(i)} - \epsilon_m^{(i)})$ is satisfied for every n and m [55].

Let assume that a temperature T_A exists such that $\hat{\rho}_A = \hat{\rho}_G[\lambda_f, T_A]$ (we will consider the more general case later). Similarly to the irreversible work $\langle w_{irr}\rangle$, the inner friction can then be expressed in terms of the quantum relative entropy of the state $\hat{\rho}_\tau$ with respect to the state $\hat{\rho}_A$ by

$$\langle w_{fric}\rangle = \beta_A^{-1} D(\hat{\rho}_\tau || \hat{\rho}_A) \tag{27}$$

If we think in terms of heat transfer, the inner friction is the amount of work lost if the end state $\hat{\rho}_\tau$ is not the equilibrium state $\hat{\rho}_A$. If the system is kept in contact with a heat bath at the temperature T_A after it reaches the state $\hat{\rho}_\tau$, it will take from the bath the heat $\langle Q^{th}_{\tau\to A}\rangle = -\langle w_{fric}\rangle$ in order to go to the equilibrium thermal state $\hat{\rho}_A$.

The inner friction and the irreversible work can be related by the equation

$$\langle w_{irr}\rangle - \langle w_{fric}\rangle = \mathcal{U}_A - \mathcal{U}_B - T_i(S_A - S_B) \tag{28}$$

where $\mathcal{U}_A$ and $\mathcal{U}_B$ are the internal energies of the equilibrium states $\hat{\rho}_A$ and $\hat{\rho}_B$ respectively. From the Eq. (28), we see that the two quantities are equal $\langle w_{fric}\rangle = \langle w_{irr}\rangle$, for a cyclic process or in the limit of zero temperatures[3] .

From a thermodynamic point of view, the out of equilibrium process differs from the reversible adiabatic process, because of a production of entropy due to the non adiabatic transitions occurring in the irreversible transformation. There are different suggestions to characterize the thermodynamic entropy of a generic quantum state [56, 57].

By following [16], we introduce the stochastic variable s

$$s = \beta_A \epsilon_n^{(f)} - \beta_i \epsilon_m^{(i)} \tag{29}$$

having the probability distribution

$$p(s) = \sum_{n,m} P_m^{(i)} P_{m\to n}(\tau) \delta\left(s - \beta_A \epsilon_n^{(f)} + \beta_i \epsilon_m^{(i)}\right) \tag{30}$$

3 In the limiting case of zero temperatures, these two reversible transformations of reference coincide. Instead for a cyclic process, the two final equilibrium states coincide $\rho_A = \rho_B$. Then, in both cases $\langle w_{fric}\rangle = \langle w_{irr}\rangle$.

The fluctuations of s are constrained by the Tasaki fluctuation theorem

$$\langle e^{-s}\rangle = \sum_{n,m} P_m^{(i)} P_{m\to n}(\tau) e^{\beta_A \epsilon_n^{(f)} - \beta_i \epsilon_m^{(i)}} = \frac{Z_A}{Z_i} \tag{31}$$

The free energies at the two thermal equilibrium states $\hat{\rho}_A$ and $\hat{\rho}_i$ are related to the partition functions by $F_A = -\ln(Z_A)/\beta_A$ and $F_i = -\ln(Z_i)/\beta_i$ respectively. The entropies can be expressed as $S_A = \beta_A \mathcal{U}_A - \beta_A F_A$ and $S_i = \beta_i \mathcal{U}_i - \beta_i F_i$, then the quantity

$$\begin{aligned} \langle \Sigma \rangle &= \langle s \rangle - \beta_A F_A + \beta_i F_i && (32) \\ &= \beta_A (\mathrm{Tr}\left\{\hat{H}_f \hat{\rho}_\tau\right\} - F_A) - \beta_i(\mathcal{U}_i - F_i) && (33) \end{aligned}$$

can be interpreted as the entropy produced in the process, and Σ satisfies the fluctuation theorem

$$\langle e^{-\Sigma}\rangle = 1 \tag{34}$$

from which, for instance, it follows that $\langle \Sigma \rangle \geq 0$.

If the process is reversible, then $\langle \Sigma \rangle$ is zero because $S_A = S_i$. The entropy $\langle \Sigma \rangle$ is related to the inner friction by

$$\langle \Sigma \rangle = \beta_A \langle w_{fric} \rangle \tag{35}$$

We observe that Σ is invariant under a shift of the energy reference point, and so it is independent of the choice of the gauge [10]. If it is possible to choose the ground state energies as the energy reference point, that is $\epsilon_1^{(f)} = \epsilon_1^{(i)} = 0$, we have that $\beta_A = \beta_i \epsilon_n^{(i)} / \epsilon_n^{(f)}$ [55] and so $\beta_A F_A = \beta_i F_i$ and $s = \Sigma$.

The concepts discussed above are briefly illustrated in two simple physical systems: a quantum harmonic oscillator in Sec. 3.2.1 and a spin 1/2 in Sec. 3.2.2.

3.2.1 A Quantum Harmonic Oscillator

We consider a quantum harmonic oscillator having frequency ω.

The out of equilibrium process is generated by changing the frequency from the initial value ω_i at the time $t = 0$, to the final value ω_f at the time $t = \tau$, so that $\omega(t)$ is its value at the time t. The work stastics of this process was studied in [58], and in [59], the irreversible work was connected with the degree of squeezing of the state.

Here we compare the actual process to the ideal adiabatic one, in which the system will reach the final equilibrium state at the temperature $T_A = T_i\omega_f/\omega_i$.

The inner friction $\langle w_{fric}\rangle$ can be written as $\langle w_{fric}\rangle = \langle \delta n\rangle\omega_f$, where $\langle \delta n\rangle$ is the average number of the non adiabatic excitations generated in the process. It reads

$$\langle \delta n\rangle = \frac{Q^* - 1}{2}\coth\left(\frac{\beta_i\omega_i}{2}\right) \tag{36}$$

where Q^* is the parameter introduced in [60], and recently discussed in [58]. This parameter is intimately related to the adiabaticity of the evolution, in particular in the adiabatic limit it is $Q^* = 1$.

No excitations are generated in the adiabatic limit, and so $P_{m\to n}(\tau) = \delta_{m,n}$.

Including the first non-zero correction in the time-adiabatic perturbation expansion [53], we find the non zero transition probabilities

$$P_{m\to m\pm 2}(\tau) \simeq \frac{1}{4}\left\{\begin{array}{c}(m+1)(m+2)\\ m(m-1)\end{array}\right\}\left|\int_0^\tau \frac{e^{i2\int_0^t \omega(t')dt'}}{2\omega(t)}\frac{d\omega(t)}{dt}dt\right|^2 \tag{37}$$

that depend on how slow the frequency $\omega(t)$ is changed by its logarithmic derivative.

In this approximation, the propability of permanence in each m-state is $P_{m\to m}(\tau) \simeq 1 - P_{m\to m+2}(\tau) - P_{m\to m-2}(\tau)$.

By using the expressions in Eq. (37), we find

$$\langle \delta n\rangle \simeq \coth\left(\frac{\beta_i\omega_i}{2}\right)\left|\int_0^\tau \frac{e^{i2\int_0^t \omega(t')dt'}}{2\omega(t)}\frac{d\omega(t)}{dt}dt\right|^2 \tag{38}$$

For a non adiabatic time-evolution, the transition probabilities $P_{m\to n}(\tau)$ can be calculated from the generating function given in [60].

3.2.2 A Landau-Zener Process

Another fundamental system to which we can easily apply the general theoretical considerations developed above, is a spin 1/2 particle in presence of a time-dependent magnetic field. The spin is described by the operators $\hat{\boldsymbol{S}} = (\hat{S}^x, \hat{S}^y, \hat{S}^z)$, satisfying the commutation relations

$$\left[\hat{S}^\alpha, \hat{S}^\beta\right] = i \sum_\gamma \mathcal{E}_{\alpha\beta\gamma} \hat{S}^\gamma$$

where $\mathcal{E}_{\alpha\beta\gamma}$ is the Levi-Civita symbol. The spin operators are expressed in terms of the Pauli matrices $\hat{\boldsymbol{\sigma}} = (\hat{\sigma}^x, \hat{\sigma}^y, \hat{\sigma}^z)$ by $\hat{\boldsymbol{S}} = \frac{1}{2}\hat{\boldsymbol{\sigma}}$.

We assume to reverse the direction of the magnetic field by changing its intensity linearly in time. The crossing in the energy levels is avoid by taking into account a little perturbation in the Hamiltonian, so that the system is described by the Landau-Zener Hamiltonian [61, 62]

$$\hat{H}(B) = -B\hat{\sigma}^z + \epsilon\hat{\sigma}^x \tag{39}$$

where the parameter B is changed from the initial value $B_i = -B_0$ to $B_f = B_0$, in the time interval $[-\tau, \tau]$, following the protocol $B(t) = vt$, so that $B_0 = v\tau > 0$. It is assumed that $\epsilon \ll B_0$, so that a spin flip can occur only as $t \sim 0$.

We consider the case in which the field is initially strong enough, so that the initial state of the spin is the ground state $|\downarrow\rangle$. Then if the initial temperature is T_i, we require that $B_0 \gg k_B T_i$.

If the parameter is changed adiabatically, i.e. in the limit $v \to 0$, the spin adiabatically follows the direction of the magnetic field, reaching the final state $|\uparrow\rangle$, and the work done in this reversible process is zero.

For a finite speed v, we have an increase of internal energy by a production of irreversible work $\langle w_{irr}\rangle = \langle w_{fric}\rangle = \langle w\rangle$.

In the limit $B_0 \to \infty$, the asymptotic limit of the irreversible work can be calculated as in [63], obtaining

$$\langle w_{irr}\rangle \sim 2B_0 e^{-\frac{\pi\epsilon^2}{v}} \tag{40}$$

Then, as the process tends to be slow, the irreversible work done goes exponentially to zero.

3.3 NON-ADIABATICITY, WORK AND QUANTUM COHERENCE

The existence of a unitary process for which the state $\hat{\rho}_A$ is a thermal Gibbs state $\hat{\rho}_G[\lambda_f, T_A]$, plays a relevant role in thermodynamics, but it is also a tight requirement [55]. It can be achieved in paradigmatic quantum systems such as a two level system or a harmonic oscillator, but not in all quantum systems.

So, in general the inner friction $\langle w_{fric} \rangle$ is not related to the quantum relative entropy $D(\hat{\rho}_\tau || \hat{\rho}_A)$ by the Eq. (27). Anyway, the "entropic measure"

$$\mathcal{N}_A = D(\hat{\rho}_\tau || \hat{\rho}_A) \tag{41}$$

can still be used to quantify the non adiabaticity of the evolution. It is related to the work done $\langle w \rangle$ by the equality

$$\mathcal{N}_A = \beta_i \left(\langle w \rangle + \langle \tilde{w}_{ad} \rangle \right) \tag{42}$$

where $\langle \tilde{w}_{ad} \rangle$ is the work done in an ideal process in which we try to come back to the initial state $\hat{\rho}_i$, starting from the final state $\hat{\rho}_\tau$, by using an adiabatic time reversed process.

If the microreversibility principle holds [10], the wanted time reversed process is achieved when the parameter λ adiabatically retraces its history in time. Otherwise, it is obtained by the time reversed evolution $\hat{U}_A^\dagger$ (see App. 3.A).

During the change of the parameter λ, the state of the system is typically unable to follow perfectly the equilibrium state, as signaled by a non zero $\mathcal{N}_A$.

This inability is a consequence of both the creation of non zero coherences, and the change of the populations, with respect to the reference basis of the instantaneous eigenstates of the Hamiltonian. These two contributions can be isolated in $\mathcal{N}_A$

$$\mathcal{N}_A = C(\hat{\rho}_\tau) + D(\hat{\Delta}(\hat{\rho}_\tau)||\hat{\rho}_A) \tag{43}$$

where $C(\hat{\rho}_\tau)$ is the relative entropy of coherence [64, 65], defined by

$$C(\hat{\rho}_\tau) = D(\hat{\rho}_\tau||\hat{\Delta}(\hat{\rho}_\tau)) \tag{44}$$

and so the contribution coming from the change in populations is given by $D(\hat{\Delta}(\hat{\rho}_\tau)||\hat{\rho}_A)$. The dephasing operator $\hat{\Delta}$ is defined by Eq. (15) by choosing the reference basis $\{\left|\epsilon_n^{(f)}\right\rangle\}_n$.

Eq. (43) can be obtained by using the mathematical identity [4]

$$D(\hat{\rho}||\hat{\sigma}) = C(\hat{\rho}) + D(\hat{\Delta}(\hat{\rho})||\hat{\sigma}) \tag{45}$$

where $\hat{\rho}$ is an arbitrary density matrix, and the density matrix $\hat{\sigma}$ is such that $\hat{\Delta}(\hat{\sigma}) = \hat{\sigma}$.

If is possible to consider an adiabatic perturbation expansion of $\hat{U}_{\tau,0}[\lambda]$ in the adiabatic parameter τ^{-1}, then at the second order in τ^{-1} it follows [5]

$$\mathcal{N}_A \simeq C(\hat{\rho}_\tau) \tag{46}$$

If $\hat{\rho}_A$ is the thermal equilibrium state $\hat{\rho}_G[\lambda_f, T_A]$, the measure $\mathcal{N}_A$ can be recognized as the entropy produced $\langle\Sigma\rangle$. This means that as we start to go away from the reversible adiabatic process, the production of entropy $\langle\Sigma\rangle$ starts because of the generation of coherences in the state $\hat{\rho}_\tau$.

A relation analogous to the Eq. (43) is obtained for the irreversible work as well

$$\langle w_{irr}\rangle = \beta_i^{-1}\left(C(\hat{\rho}_\tau) + D(\hat{\Delta}(\hat{\rho}_\tau)||\hat{\rho}_B)\right) \tag{47}$$

and by using $\langle w_{irr}\rangle = \langle w\rangle - \Delta F$, it follows that

$$C(\hat{\rho}_\tau) = \beta_i\langle w_{irr}\rangle + \beta_i\left(\langle\tilde{w}_{ad}\rangle + \Delta F\right) - D(\hat{\Delta}(\hat{\rho}_\tau)||\hat{\rho}_A) \tag{48}$$

In a cyclic process, the final Hamiltonian is equal to the initial one $\hat{H}_f = \hat{H}_i$, and so

4 See App. 3.B for a proof.

5 See App. 3.C for a proof.

$$\langle w\rangle = \beta_i^{-1}\left(C(\hat{\rho}_\tau) + D(\hat{\Delta}(\hat{\rho}_\tau)||\hat{\rho}_i)\right) \tag{49}$$

3.4 SUMMARY AND CONCLUSIONS

We have discussed the thermodynamic work done in out of equilibrium processes, assuming that the system can be considered closed during the driving. The discussion is carried on by taking into account the irreversible amount of work produced in the process, which can be quantified in terms of either the inner friction $\left\langle w_{fric}\right\rangle$ or the irreversible work $\langle w_{irr}\rangle$, depending on the reversible transformation that is taken as a reference. These two figures of merit are linked to the quantum relative entropy and to the heat that is exchanged in a thermalization process. Furthermore, the thermodynamic work has been related to the distance of the real process from an ideal quantum adiabatic one. This is obtained by considering an "entropic" measure of the non adiabaticity of the process, investigating also the case of a quasi-adiabatic approximation for the process. The role played by the quantum coherence, generated in the process, is also briefly discussed.

APPENDICES

3.A RELATION BETWEEN $\mathcal{N}_A$ AND THE WORK

In this Appendix we describe the time reverse process discussed in Sec. 3.3, proving the relation in Eq. (42) of Sec. 3.3, that connects the work to the non adiabaticity of the out of equilibrium process quantified by the entropic measure $\mathcal{N}_A$ defined in Eq. (41).

The out of equilibrium process $\hat{\rho}_i \mapsto \hat{\rho}_\tau$ is described by the time evolution $\hat{U}_{t,0}[\lambda]$, and its time-reversed evolution from τ to t, is described by $\hat{U}^\dagger_{\tau,t}[\lambda]$, generated by the time-reversed Hamiltonian. Under the assumption that at any time t the Hamiltonian is invariant under the time-reversal operation $\hat{\Theta}$, that is $\hat{\Theta}\hat{H}(\lambda(t)) = \hat{H}(\lambda(t))\hat{\Theta}$, we can consider a time-reversed process having time evolution operator $\hat{U}_{t,0}[\tilde{\lambda}] = \hat{\tilde{U}}_{t,0}[\lambda]$, where $\tilde{\lambda}(t) = \lambda(\tau - t)$, since the principle of microreversibility, expressed as

$$\hat{U}_{\tau-t,0}[\tilde{\lambda}]\hat{\Theta} = \hat{\Theta}\hat{U}_{t,\tau}[\lambda] = \hat{\Theta}\hat{U}^\dagger_{\tau,t}[\lambda] \tag{50}$$

holds, as shown in [10].

Indeed, if the energy spectrum is non degenerate, from the Eq. (50) it follows that

$$\left|\left\langle \epsilon^{(i)}_m \right| \hat{U}_{\tau,0}[\tilde{\lambda}] \left| \epsilon^{(f)}_n \right\rangle\right| = \left|\left\langle \epsilon^{(i)}_m \right| \hat{U}^\dagger_{\tau,0}[\lambda] \left| \epsilon^{(f)}_n \right\rangle\right| \tag{51}$$

The operator $\hat{\tilde{U}}_A$ is defined as the adiabatic limit of the operator $\hat{U}_{\tau,0}[\tilde{\lambda}]$, and analogously to the operator $\hat{U}_A$, the state $\hat{\tilde{U}}_A \left| \epsilon^{(f)}_n \right\rangle$ differs from $\left| \epsilon^{(i)}_n \right\rangle$ only by a global phase.

Then the work done in the adiabatic time-reversed process is by definition

$$\langle \tilde{w}_{ad} \rangle = \mathrm{Tr}\left\{\hat{H}_i \hat{\tilde{U}}_A \hat{\rho}_\tau \hat{\tilde{U}}^\dagger_A\right\} - \mathrm{Tr}\left\{\hat{H}_f \hat{\rho}_\tau\right\} \tag{52}$$

from which

$$\langle \tilde{w}_{ad} \rangle = \sum_n \epsilon^{(i)}_n \left\langle \epsilon^{(i)}_n \right| \hat{\tilde{U}}_A \hat{\rho}_\tau \hat{\tilde{U}}^\dagger_A \left| \epsilon^{(i)}_n \right\rangle - \epsilon^{(f)}_n P_n(\tau) \tag{53}$$

Since $\hat{\tilde{U}}_A \left| \epsilon^{(f)}_n \right\rangle$ differs from $\left| \epsilon^{(i)}_n \right\rangle$ only by a global phase, it is easy to show that

$$\langle \tilde{w}_{ad} \rangle = \sum_n P_n(\tau)\left(\epsilon_n^{(i)} - \epsilon_n^{(f)}\right) \tag{54}$$

If time reversal symmetry does not hold, we have to use $\hat{U}_A^\dagger$ instead of $\hat{\tilde{U}}_A$, but the expression obtained for $\langle \tilde{w}_{ad} \rangle$ remains unchanged.

By using the definition of $\langle w \rangle$, we have

$$\begin{aligned}
\beta_i\left(\langle w \rangle + \langle \tilde{w}_{ad} \rangle\right) &= \sum_n (P_n(\tau) - P_n^{(i)})\beta_i \epsilon_n^{(i)} \\
&= \sum_n (P_n^{(i)} - P_n(\tau)) \ln P_n^{(i)} \\
&= \sum_n P_n^{(i)} \ln P_n^{(i)} - \sum_n P_n(\tau) \ln P_n^{(A)} \\
&= -S(\hat{\rho}_i) - \mathrm{Tr}\left\{\hat{\rho}_\tau \ln \hat{\rho}_A\right\} \\
&= -S(\hat{\rho}_\tau) - \mathrm{Tr}\left\{\hat{\rho}_\tau \ln \hat{\rho}_A\right\} \\
&= D(\hat{\rho}_\tau || \hat{\rho}_A)
\end{aligned}$$

that is the Eq. (42) of Sec. 3.3.

3.B A MATHEMATICAL IDENTITY

In this Appendix we show the mathematical identity in Eq. (45) of Sec. 3.3, that has been used to prove Eq. (43) and Eq. (47). Given an arbitrary state $\hat{\rho}$ and a state $\hat{\sigma}$ that is diagonal in the basis of reference that defines the dephasing operator $\hat{\Delta}$, the quantum relative entropy $D(\hat{\rho}_1||\hat{\rho}_2)$ defined in Eq. (23), can be decomposed as the sum of two contributions. The first one is due to the coherences in $\hat{\rho}$, the second to the population difference between $\hat{\Delta}(\hat{\rho})$ and $\hat{\sigma}$. Explicitly

$$\begin{aligned}
D(\hat{\rho}||\hat{\sigma}) &= -S(\hat{\rho}) - \mathrm{Tr}\left\{\hat{\rho} \ln \hat{\sigma}\right\} \\
&= -S(\hat{\rho}) + S(\hat{\Delta}(\hat{\rho})) - S(\hat{\Delta}(\hat{\rho})) - \mathrm{Tr}\left\{\hat{\rho} \ln \hat{\sigma}\right\} \\
&= C(\hat{\rho}) - S(\hat{\Delta}(\hat{\rho})) - \mathrm{Tr}\left\{\hat{\rho} \ln \hat{\sigma}\right\}
\end{aligned}$$

Explicitly the dephasing operator can be expanded as $\hat{\Delta}\hat{\rho} = \sum_n \langle \epsilon_n | \hat{\rho} | \epsilon_n \rangle | \epsilon_n \rangle \langle \epsilon_n |$. The operator $\hat{\sigma}$ is diagonal in the basis $\{|\epsilon_n\rangle\}_n$ which defines the dephasing, hence only the diagonal part of the density matrix ρ counts for the trace, and so

$$\begin{aligned} D(\hat{\rho}||\hat{\sigma}) &= C(\hat{\rho}) - S(\hat{\Delta}(\hat{\rho})) - \mathrm{Tr}\left\{\hat{\Delta}(\hat{\rho}) \ln \hat{\sigma}\right\} \\ &= C(\hat{\rho}) + D(\hat{\Delta}(\hat{\rho})||\hat{\sigma}) \end{aligned}$$

where $C(\hat{\rho})$ is the quantum coherence measure defined in (44), that is found to be equal to $C(\hat{\rho}) = S(\hat{\Delta}(\hat{\rho})) - S(\hat{\rho})$ [65].

3.C ADIABATIC PERTURBATION EXPANSION

In this Appendix, we prove the relation in Eq. (46) of the Sec. 3.3, that shows how the quantum non adiabaticity of a process, quantified by $\mathcal{N}_A$, is related to the quantum coherence, as the process becomes "quasi-adiabatic".

In the adiabatic approximation, the transition probability is $P_{m\to n}(\tau) \to \delta_{m\,n}$.

If non-adiabatic transitions are taken into account by performing an adiabatic perturbation expansion [53], there can be a corrections, so that the transition probability is

$$P_{m\to n}(\tau) \simeq \delta_{m\,n} + P^{(2)}_{m\to n}(\tau) \tag{55}$$

Let us focus on the entropy $S(\hat{\Delta}(\hat{\rho}_\tau))$. By using this approximation we have

$$
\begin{aligned}
S(\hat{\Delta}(\hat{\rho}_\tau)) &= -\sum_n P_n(\tau) \ln P_n(\tau) \\
&\simeq -\sum_n P_n(\tau) \ln \left(P_n^{(i)} + \sum_m P_m^{(i)} P_{m\to n}^{(2)}(\tau) \right) \\
&\simeq -\sum_n P_n(\tau) \ln P_n^{(i)} - \\
&\quad \sum_n P_n(\tau) \ln \left(1 + \sum_m \frac{P_m^{(i)}}{P_n^{(i)}} P_{m\to n}^{(2)}(\tau) \right) \\
&\simeq -\sum_n P_n(\tau) \ln P_n^{(i)} - \sum_n \sum_m P_m^{(i)} P_{m\to n}^{(2)}(\tau)
\end{aligned}
$$

The second order transition probabilities $P_{m\to n}^{(2)}(\tau)$ are such that $\sum_n P_{m\to n}^{(2)}(\tau) = 0$, because $\sum_n P_{m\to n}(\tau) = 1$. Then

$$
\begin{aligned}
S(\hat{\Delta}(\hat{\rho}_\tau)) &\simeq -\sum_n P_n(\tau) \ln P_n^{(i)} \\
&= -\sum_n P_n(\tau) \ln P_n^{(A)} \\
&= -\mathrm{Tr}\left\{ \hat{\rho}_\tau \ln \hat{\rho}_A \right\}
\end{aligned}
$$

and so

$$
\begin{aligned}
\mathcal{N}_A &= -S(\hat{\rho}_\tau) - \mathrm{Tr}\left\{ \hat{\rho}_\tau \ln \hat{\rho}_A \right\} \\
&= -S(\hat{\rho}_i) - \mathrm{Tr}\left\{ \hat{\rho}_\tau \ln \hat{\rho}_A \right\} \\
&\simeq -S(\hat{\rho}_i) + S(\hat{\Delta}(\hat{\rho}_\tau)) \\
&= C(\hat{\rho}_\tau)
\end{aligned}
$$

4 WORK EXTRACTION AND QUANTUM CORRELATIONS

In this Chapter, we examine the possibility to infer about the existence of quantum correlations, by looking at the thermodynamics of an out of equilibrium process [E]. This study is carried out for a general finite dimensional quantum system, by considering a suitable work extraction protocol.

The conventional process of work extraction from a storing center that is a closed quantum system, is discussed in Sec. 4.1 in terms of the quantum *ergotropy* [66]. The ergotropy is defined as the maximum amount of work extractable from the system, by means of a unitary cycle, and plays a key role in charging the storing center [67, 68]. There, it is also shown how the contribution given to the ergotropy by the quantum coherence, can be easily identified when the system is first prepared in some special states.

In Sec. 4.2 we consider a bipartite quantum system, and we show how it is possible to optimize the process of work extraction, by using a suitable feedback protocol. The protocol enhances the work extraction procedure, by taking advantage of the initial correlations between the two parts of the system. The maximum *daemonic gain* achieved is strictly related to the quantum nature of the correlations. In general, it behaves as a witness for quantum correlation, and defines a thermodynamic criterion for separability, that is necessary and sufficient for bipartite pure states. Furthermore, an explicit example with a simple system of two qubits is considered in Sec. 4.2.1, where the daemonic gain is related to the quantum correlations between the two qubits. Explicitly, we give a characterization of the states which, for a given value of gain, maximize the quantum correlations. We take into account both the correlations as measured by the discord, and those quantified by the concurrence.

4.1 WORK EXTRACTION FROM FINITE QUANTUM SYSTEMS

The possibility to realize small heat engines, has recently received a great deal of attention from the scientific community. In this scenario, a quantum system S can play the role of a storing center (a so-called quantum battery) [69], i.e. it can be used to temporarily store energy that will be later extracted in order to perform some useful work (for instance, the driving of a small heat engines [70]).

When the work is extracted from the system S by permorming a cyclic process during which the system is thermally isolated from its environment, the ergotropy [66], defined as the maximum amount of work extractable from the system by using an unitary cycle, becomes a key quantity. Ideally, the system S is characterized by its initial state $\hat{\rho}$ and its Hamiltonian $\hat{H}$, and the cyclic process is realized by manipulating some external fields (work parameters) that are switched on only in the time interval $[0, \tau]$ [69], so that the time evolution $\hat{U}_{t,0}$ in this interval is generated by the Hamiltonian $\hat{H}(t) = \hat{H} + \hat{V}(t)$ where $\hat{V}(t)$ is such that $\hat{V}(0) = \hat{V}(\tau) = 0$.

Since the system is closed, it will reach the final state $\hat{\rho}_\tau = \hat{U}_{\tau,0}\hat{\rho}\hat{U}^\dagger_{\tau,0}$ at time $t = \tau$, and the amount of work extracted W_{ex} will be equal to its average energy decrease

$$W_{ex} = \mathrm{Tr}\left\{\hat{H}\hat{\rho}\right\} - \mathrm{Tr}\left\{\hat{H}\hat{\rho}_\tau\right\}$$

There are states, called passive states, from which no work can be extracted, that is $W_{ex} = 0$ for every time function $\hat{V}(t)$ that satisfies the conditions $\hat{V}(0) = \hat{V}(\tau) = 0$. An example of a passive state is a thermal Gibbs state (21). A non passive state can be achieved by considering a bipartite system S, with the two parts prepared in thermal equilibrium states at different temperatures.

The work extracted W_{ex} cannot be larger than $\mathcal{W}_{th} = \mathrm{Tr}\left\{\hat{H}(\hat{\rho} - \hat{\rho}_{th})\right\}$, where the passive state $\hat{\rho}_{th}$ is the thermal Gibbs state at the temperature T defined by the equation $S(\hat{\rho}_{th}) = S(\hat{\rho})$ [66, 69].

For a two level system, it is always possible to perform a unitary and to reach the final state $\hat{\rho}_{th}$ (the unitary is the one that diagonalizes the initial density matrix $\hat{\rho}$), but this is not true in general. For this reasons, the concept of ergotropy $\mathcal{W}$ has been introduced as the maximum amount of work (optimized over all the possible cyclic processes defined above) that can be extracted from the system S having Hamiltonian $\hat{H}$ and prepared in the initial state $\hat{\rho}$. The ergotropy can be expressed as [66]

$$\mathcal{W} = \sum_k \sum_j r_k \epsilon_j \left(|\langle \epsilon_j | r_k \rangle|^2 - \delta_{j\,k} \right) \tag{56}$$

where we have considered

$$\hat{H} = \sum_k \epsilon_k \left|\epsilon_k\right\rangle \left\langle\epsilon_k\right| \;, \quad \hat{\rho} = \sum_k r_k \left|r_k\right\rangle \left\langle r_k\right| \tag{57}$$

with the eigen-energies ϵ_k and the populations r_k ordered such that $\epsilon_k \leq \epsilon_{k+1}$ and $r_k \geq r_{k+1}$. The ergotropy $\mathcal{W}$ is a non negative quantity, and we have $\mathcal{W} = 0$ if and only if the initial state $\hat{\rho}$ is a passive state [69]. The work extracted W_{ex} is equal to $\mathcal{W}$ if and only if the final state reached thanks to the unitary $\hat{U}_{\tau,0}$ is a passive state. Of course, if there are degeneracies in the energy spectrum, there is not a unique passive state unitarily connected to $\hat{\rho}$.

Clearly, the ergotropy cannot be greater than $\mathcal{W}_{th}$ [66]. In general, the limit $\mathcal{W}_{th}$ is asymptotically achievable by considering an infinite number of copies of the system S [69].

When the state ρ is unitarily connected to a passive thermal Gibbs state $\hat{\sigma}_\beta = e^{-\beta\hat{H}}/Z$, then the ergotropy is equal to $\mathcal{W}_{th}$, and it is given by $\mathcal{W} = \mathrm{Tr}\left\{\hat{H}(\hat{\rho} - \hat{\sigma}_\beta)\right\}$. In this case, from the Eq. (49), it follows that

$$\mathcal{W} = \beta^{-1} \left(C(\hat{\rho}) + D(\hat{\Delta}(\hat{\rho})||\hat{\sigma}_\beta) \right) \tag{58}$$

where $\hat{\Delta}$ is the dephasing operator with respect to the basis of the eigenstates of $\hat{H}$. In Eq. (58), the quantum contribution given by the coherences, characterized by the coherence measure $C(\hat{\rho})$, is separated from the "classical" contribution to the ergotropy $\mathcal{W}$, given by $D(\hat{\Delta}(\hat{\rho})||\hat{\sigma}_\beta)$, which is due to the population differences.

Those states $\hat{\rho}$ for which $\hat{\Delta}(\hat{\rho}) = \hat{\sigma}_\beta$ give the ergotropy $\mathcal{W} = \beta^{-1} C(\hat{\rho})$.

4.2 DAEMONIC ERGOTROPY

In order to connect the ergotropy with the theory of quantum correlations, we extend this maximal work extraction framework by introducing a non-interacting ancilla A and assume that the system S, playing the role of storing center, and the ancilla A are initially prepared in the joint state $\hat{\rho}_{SA}$. The intuition behind the protocol, that will be discussed below, is that should $\hat{\rho}_{SA}$ bring about correlations between S and A, a measurement performed on the ancilla would give us information about the state of S, which could then be used to enhance the amount of work that can be extracted from its state.

The correlations between the system and the ancilla can be generated without changing the average energy of the storing center S. For instance, the state ρ_{SA} can be achieved starting from a global state with no correlations, by engineering an interaction between S and A of the kind $\hat{V}_{SA}(t) = \sum_k |\epsilon_k\rangle \langle\epsilon_k|_S \otimes \hat{A}_k(t)$. The states $|\epsilon_k\rangle_S$ are the eigenstates of the Hamiltonian of S, and the operators $\hat{A}_k(t)$ act on the Hilbert space of the ancilla A, and change in time so that at the end of such protocol the two systems do not interact with each other anymore.

For our purposes, we focus on the case in which the work is extracted by local unitary cycles on the part S: i.e. we assume that S and A do not interact with each other, and control the parameters of the system S, so that at the end its Hamiltonian is equal to the initial one, that we indicate with $\hat{H}_S$

$$\hat{H}_S = \sum_k \epsilon_k |\epsilon_k\rangle \langle\epsilon_k|_S \ , \quad \epsilon_k \leq \epsilon_{k+1}$$

We assume to be able to perform a Von Neumann measurement on the state of the ancilla A. This kind of measurement can be described by a set of orthogonal projectors of rank one $\{\hat{\Pi}_a^A = |a\rangle \langle a|_A\}_a$. Specifically the state of the system S collapses into the density matrix $\hat{\rho}_{S|a} = \mathrm{Tr}_A \left\{ \hat{\mathbb{1}}_S \otimes \hat{\Pi}_a^A \hat{\rho}_{SA} \right\} / p_a$, with the probability $p_a = \text{Tr}\left\{\hat{\Pi}_a^A \hat{\rho}_{SA}\right\}$. The post measurement density matrix can be written as

$$\hat{\rho}_{S|a} = \sum_k r_k^a \left|r_k^a\right\rangle \left\langle r_k^a\right|_S \;, \quad r_k^a \geq r_{k+1}^a$$

The time evolution of state $\hat{\rho}_{S|a}$ then follows a cyclic unitary process $\hat{U}_a$ conditioned on the outcome of the measurement. By averaging over all of the possible measurement outcomes, the work extracted from the state of S reads

$$W_{\{\Pi_a^A\}} = \text{Tr}\left\{\hat{\rho}_S \hat{H}_S\right\} - \sum_a p_a \text{Tr}\left\{\hat{U}_a \hat{\rho}_{S|a} \hat{U}_a^\dagger \hat{H}_S\right\}$$

Since $\text{Tr}\left\{\hat{\rho}_S \hat{H}_S\right\} = \sum_a p_a \text{Tr}\left\{\hat{\rho}_{S|a} \hat{H}_S\right\}$, and $\text{Tr}\left\{\hat{\rho}_{S|a} \hat{H}_S\right\} - \text{Tr}\left\{\hat{U}_a \hat{\rho}_{S|a} \hat{U}_a^\dagger \hat{H}_S\right\}$ is smaller than the ergotropy of the state $\hat{\rho}_{S|a}$ calculated with respect to the Hamiltonian $\hat{H}_S$, which is given by $\text{Tr}\left\{\hat{H}_S \hat{\rho}_{S|a}\right\} - \sum_k r_k^a \epsilon_k$, we have that the work $W_{\{\hat{\Pi}_a^A\}}$ cannot be larger than the quantity

$$\mathcal{W}_{\{\hat{\Pi}_a^A\}} = Tr\{\hat{\rho}_S \hat{H}_S\} - \sum_a p_a \sum_k r_k^a \epsilon_k \tag{59}$$

This quantity is obtained by a maximization of the work $W_{\{\hat{\Pi}_a^A\}}$ over all the possible ways to control the system S, and we call it *Daemonic Ergotropy*, because it depends by the amount of information about S extracted from A.

If we do not use the information obtained upon measuring the ancilla, and thus control the system S in the same way, independently of the measurement outcomes , so that $\hat{U}_a = \hat{U}$ for every a, the maximum extractable work would be given by the ergotropy $\mathcal{W}$ associated with state $\hat{\rho}_S = Tr_A\{\hat{\rho}_{SA}\} = \sum_a p_a \hat{\rho}_{S|a}$.

If

$$\hat{\rho}_S = \sum_k r_k \left|r_k\right\rangle \left\langle r_k\right| \;, \quad r_k \geq r_{k+1}$$

then the ergotropy reads

$$\mathcal{W} = Tr\{\hat{\rho}_S \hat{H}_S\} - \sum_k r_k \epsilon_k \tag{60}$$

In App. 4.A, we show that the information acquired through the measurements allows to extract more work than in the absence of them, that is $\mathcal{W}_{\{\hat{\Pi}_a^A\}} \geq \mathcal{W}$ and that it provides an upperbound on the ergotropy.

The characterization of the efficiency of this work extraction scheme, though, should take into account the energetic cost of the measurements ΔE_{meas}, whose quantification depends on several factors. However, it cannot be smaller than the average variation in the energy of A, so that a lower value can be established as $\Delta E_{\text{meas}} \geq \sum_a p_a \text{Tr}\left\{\hat{\Pi}_a^A \hat{H}_A\right\} - \text{Tr}\left\{\hat{H}_A \hat{\rho}_A\right\}$ with $\hat{H}_A$ the Hamiltonian of the ancilla and $\hat{\rho}_A = \text{Tr}_S\{\hat{\rho}_{SA}\}$ its reduced state.

For our purposes, the main object of our attention will be the difference $\mathcal{W}_{\{\hat{\Pi}_a^A\}} - \mathcal{W}$, since we expect it to be related to the correlations between S and A. For instance, if S and A are initially statistically independent, i.e. $\hat{\rho}_{SA} = \hat{\rho}_S \otimes \hat{\rho}_A$, then the measurements on the ancilla would not bring about any information on the state of S, as we would have $\hat{\rho}_{S|a} = \hat{\rho}_S$ for any set $\{\hat{\Pi}_a^A\}$ and outcome a.

Consequently, $\mathcal{W}_{\{\hat{\Pi}_a^A\}} = \mathcal{W}$, and there would be no gain in work extraction.

Then, it is natural to ask what happens when it is not possible to have a gain. In order to answer to this question, we consider the maximum gain

$$\delta\mathcal{W} = \max_{\{\hat{\Pi}_a^A\}} \mathcal{W}_{\{\hat{\Pi}_a^A\}} - \mathcal{W}, \tag{61}$$

and we refer to it as *daemonic gain*. Clearly, $\delta\mathcal{W} \geq 0$ because of the considerations above and the optimization entailed in Eq. (59).

Our aim is to connect $\delta\mathcal{W}$ to quantum correlations.

To this end, we notice that $\delta\mathcal{W}$ is invariant under local unitary transformations of the form $\hat{U}_S \otimes \hat{U}_A$. Indeed, any unitary transformation on S can be incorporated into the transformations used for the extraction of work, while the action of any unitary on A is equivalent to a change of the measurement basis.

We show below that $\delta\mathcal{W}$ is intimately related to the quantum correlations shared by S and A, quantified by the quantum discord [45, 46].

For projective measurements performed on the system S, discord is defined as

$$\overrightarrow{\mathcal{D}}_{SA} = \mathcal{I}_{SA} - \max_{\{\hat{\Pi}_a^S\}} \overrightarrow{\mathcal{J}}_{SA}, \tag{62}$$

where $\mathcal{I}_{SA}$ is the mutual information between S and A, and $\overrightarrow{\mathcal{J}}_{SA}$ is the one-way classical information associated with an orthogonal measurement set $\{\hat{\Pi}_a^S\}$ performed on the system [45] (see App. 4.A for details and for the explicit definitions of $\mathcal{I}_{SA}$ and $\overrightarrow{\mathcal{J}}_{SA}$).

It is possible to infer about the quantum correlations in the state ρ_{SA} by looking at the gain in the work extraction, because of the following theorem

Theorem 4.2.1 *For any system S and ancilla A prepared in a state $\hat{\rho}_{SA}$, we have*

$$\delta\mathcal{W} = 0 \Rightarrow \overrightarrow{\mathcal{D}}_{SA} = 0 \tag{63}$$

with $\delta\mathcal{W}$ and $\overrightarrow{\mathcal{D}}_{SA}$ as defined in Eq. (61) *and in Eq.* (62)*, respectively.*

The asymmetry of the daemonic gain is well reflected into the impossibility of linking $\delta\mathcal{W}$ to the discord associated with measurements performed on the ancilla. That is

$$\delta\mathcal{W} = 0 \not\Rightarrow \overleftarrow{\mathcal{D}}_{SA} = 0. \tag{64}$$

The proof of both Theorem 4.2.1 and the corollary statement in Eq. (64) are presented fully in App. 4.A. It is important to observe that, in general, the converse of Theorem 4.2.1 does not hold, i.e. $\overleftarrow{\mathcal{D}}_{SA} = 0$ or $\overrightarrow{\mathcal{D}}_{SA} = 0 \not\Rightarrow \delta\mathcal{W} = 0$ as there can well be classically correlated states associated with a non-null daemonic gain.

Instead, if $\hat{\rho}_{SA}$ is a pure state, its correlations can only be in the form of entanglement, and so from Theorem 4.2.1, $\delta\mathcal{W} = 0$ if and only if the state $\hat{\rho}_{SA}$ is separable. Specifically

Theorem 4.2.2 *For any system S and ancilla A prepared in a pure state $\hat{\rho}_{SA} = |\psi\rangle\langle\psi|_{SA}$ we have*

$$\delta\mathcal{W} = 0 \Leftrightarrow |\psi\rangle_{SA} \ \textit{is separable}, \tag{65}$$

and $\delta\mathcal{W} = \sum_k r_k \epsilon_k - \epsilon_1$, where r_k are the Schmidt coefficients of $|\psi\rangle_{SA}$ and ϵ_k are the eigenvalues of $\hat{H}_S$, ordered such that $r_k \geq r_{k+1}$ and $\epsilon_k \leq \epsilon_{k+1}$.

Theorem 4.2.2 is a thermodynamically motivated separability criterion for pure bipartite states in arbitrary dimensions and it gives an explicit quantitative link between the theory of entanglement and the thermodynamics of information.

4.2.1 Two Qubits System

The statements in Theorems 4.2.1 and 4.2.2 are completely general, and independent of the nature of either S or A, which could in principle live in Hilbert spaces of different dimensions. However, in order to illustrate their implications and gather further insight into the relation between the introduced daemonic gain and both discord and entanglement, here we focus on the smallest non-trivial situation, which is embodied by a two-qubit system.

We start with the implications of Theorem 4.2.1 and compare $\delta\mathcal{W}$ with discord $\overrightarrow{\mathcal{D}}_{SA}$. Since both these quantities are invariant under local unitary transformations on $\hat{\rho}_{SA}$, without loss of generality we can consider the system Hamiltonian $\hat{H}_S = -\hat{\sigma}_z$.

An extensive numerical analysis reveals that, for any state $\hat{\rho}_{SA}$ with a gain $\delta\mathcal{W}$, the discord $\overrightarrow{\mathcal{D}}_{SA}$, cannot be larger than

$$\mathcal{D}_{max}(\delta\mathcal{W}) = h\left(1 - \frac{\delta\mathcal{W}}{2}\right) \tag{66}$$

where $h(x) = -x\log_2(x) - (1-x)\log_2(1-x)$, as it can be seen in Fig. 4.2.1(Left Panel).

This means also that we need at least a certain amount of quantum correlations in the state $\hat{\rho}_{SA}$, quantified by $\overrightarrow{\mathcal{D}}_{SA}$, in order to be sure to have a gain $\delta\mathcal{W}$ not smaller than $\delta\mathcal{W}_{min}$, where $\delta\mathcal{W}_{min}$ is the solution of $\mathcal{D}_{max}(\delta\mathcal{W}_{min}) = \overrightarrow{\mathcal{D}}_{SA}$.

The monotonicity of $h(x)$ implies that growing values of quantum correlations are associated with a monotonically increasing daemonic gain: for the states lying on such lower bound, quantum correlations form a genuine resource for the catalysis of thermodynamic work extraction. Moreover, as $\lim_{x\to 1} h(x) =$

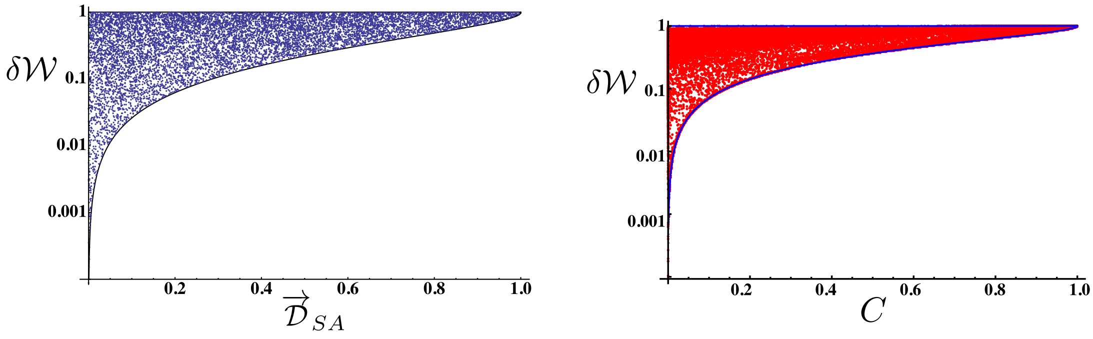

Figure 4.2.1.: (Color online): Distribution of two-qubit states in the daemonic gain-vs-discord plane (Left Panel) and in the daemonic gain-vs-concurrence plane (Right Panel). We have generated 3×10^3 general random states of system and ancilla, evaluating the daemonic gain $\delta\mathcal{W}$ and the discord $\overrightarrow{\mathcal{D}}_{SA}$ (blue dots), and the concurrence $\mathcal{C}$ (red dots) for each of them. The curves enclosing the distributions correspond to the boundaries discussed in the main text. Notice that states with no quantum correlations may correspond to arbitrarily large values of the daemonic gain $\delta\mathcal{W}$.

0, a two-qubit system with $\overrightarrow{\mathcal{D}}_{SA} = 0$ (i.e. a classically correlated state) can achieve, in principle, any value of daemonic gain up to the maximum that, for this case, is $\delta\mathcal{W} = 1$. On the other hand, the daemonic ergotropy is maximized by taking pure two-qubit states with growing degree of entanglement.

We can now address Theorem 4.2.2 and its consequences for two-qubit states. Similarly to what was done above, we have studied the distribution of random two-qubit states in the daemonic ergotropy-versus-entanglement plane, choosing quantum concurrence $\mathcal{C}$ as a measure for the latter [71]. The results are illustrated in Fig. 4.2.1(Right Panel). As before, a lower bound to the amount of daemonic ergotropy at set value of concurrence can be identified. We have that, for any state $\hat{\rho}_{SA}$ with concurrence $\mathcal{C}$

$$\delta\mathcal{W} \geq \delta\mathcal{W}_{\min}(\mathcal{C}) = 1 - \sqrt{1 - \mathcal{C}^2}, \tag{67}$$

a lower bound that is achieved by Bell-diagonal states that are fully characterized in App. 4.A.1. The upper bound, on the other hand, is achieved by maximally ergotropic (in our daemonic sense) states $\hat{\rho}_{SA} = [|00\rangle\langle 00|_{SA} + |11\rangle\langle 11|_{SA} + \mathcal{C}(|00\rangle\langle 11|_{SA} + h.c.)]/2$.

4.3 SUMMARY AND CONCLUSIONS

We have illustrated an ancilla-assisted protocol for work extraction that takes advantage of the sharing of quantum correlations between a system and an ancilla that is subjected to suitably chosen projective measurements. Our approach allowed us the introduce of a new form of information-enhanced ergotropy, which we have dubbed daemonic, which acts aptly as a witness for quantum correlations in general, and serves as a necessary and sufficient criterion for separability of bipartite pure states. We have characterised fully the distribution of quantum correlated two-qubit states with respect to the figure of merit set by the daemonic ergotropy, finding that quantum correlations embody a proper resource for the work-extraction performances at least for the states that minimize $\delta\mathcal{W}$. We are also taking into consideration the possibility to perform a similar analysis with respect to classical and total correlations. Our work opens up interesting avenues for the thermodynamic interpretation of quantum correlations, clarifies their resource-role in ancilla-assisted information thermodynamics and opens up possibilites to understand the role of correlations in the charging power of quantum batteries [67, 68].

APPENDICES

4.A DAEMONIC ERGOTROPY: PROOFS OF THE STATEMENTS

We recall the definition of quantum discord $\overleftarrow{\mathcal{D}}_{SA}$ associated with orthogonal measurements $\{\hat{\Pi}_a^A\}$ performed over the ancilla

$$\overleftarrow{\mathcal{D}}_{SA} = \mathcal{I}_{SA} - \max_{\{\hat{\Pi}_a^A\}} \overleftarrow{\mathcal{J}}_{SA}, \tag{68}$$

where $\mathcal{I}_{SA}$ is the mutual information $\mathcal{I}_{SA} = S(\hat{\rho}_A) + S(\hat{\rho}_S) - S(\hat{\rho}_{SA})$, $\overleftarrow{\mathcal{J}}_{SA} = S(\hat{\rho}_S) - \sum_a p_a S(\hat{\rho}_{S|a})$ is the so-called *one-way classical information* and $S(\hat{\rho}) = -\mathrm{Tr}\{\hat{\rho}\log_2 \hat{\rho}\}$ is the von Neumann entropy of the general state $\hat{\rho}$. The maximization inherent in Eq. (68) is over all the possible orthogonal measurements on the state of A. Similarly we define the discord $\overrightarrow{\mathcal{D}}_{SA}$ associated with measurements performed over the state of the system S as Eq. (68) with the role of S and A being swapped.

Lemma 4.A.1 *For any set of orthogonal projective measurements $\{\hat{\Pi}_a^A\}$ performed over an ancilla A prepared with a system S in a state $\hat{\rho}_{SA}$, we have $\mathcal{W}_{\{\Pi_a^A\}} \geq \mathcal{W}$*

Proof In order to show this statement, we observe that

$$\begin{aligned} \hat{\rho}_S &= \sum_k r_k \left|r_k\right\rangle \left\langle r_k\right| = \sum_a \mathrm{Tr}_A[\hat{\Pi}_a^A \hat{\rho}_{SA}] \\ &= \sum_a p_a \hat{\rho}_{S|a} = \sum_a p_a \sum_k r_k^a \left|r_k^a\right\rangle \left\langle r_k^a\right| . \end{aligned} \tag{69}$$

Eq. (69) implies that $r_k = \sum_a p_a \sum_j r_j^a |\left\langle r_k \middle| r_j^a \right\rangle|^2$.

As $\mathcal{W}_{\{\hat{\Pi}_a^A\}} - \mathcal{W} = \sum_k \epsilon_k \left(r_k - \sum_a p_a r_k^a\right)$, we have that

$$\mathcal{W}_{\{\hat{\Pi}_a^A\}} - \mathcal{W} = \sum_a p_a \sum_{k,j} r_j^a \epsilon_k \left(|\left\langle r_k \middle| r_j^a \right\rangle|^2 - \delta_{kj}\right) \geq 0 \tag{70}$$

due to the fact that $\sum_{k,j} r_j^a \epsilon_k \left(|\left\langle r_k \middle| r_j^a \right\rangle|^2 - \delta_{kj}\right) \geq 0$, as this is the ergotropy of $\hat{\rho}_{S|a}$ relative to the Hamiltonian $\sum_k \epsilon_k \left|r_k\right\rangle \left\langle r_k\right|$. ∎

Theorem 4.2.1 *For any system S and ancilla A prepared in a state $\hat{\rho}_{SA}$, we have*

$$\delta\mathcal{W} = 0 \Rightarrow \overrightarrow{\mathcal{D}}_{SA} = 0 \tag{71}$$

with $\delta\mathcal{W}$ and $\overrightarrow{\mathcal{D}}_{SA}$ as defined in Eq. (61) *and* (62)*, respectively.*

Proof In light of Lemma 4.A.1, we have that $\mathcal{W}_{\{\hat{\Pi}_a^A\}} - \mathcal{W} = 0 \Leftrightarrow \delta\mathcal{W} = 0$ for any set $\{\hat{\Pi}_a^A\}$. Then, in order to proof the statement of the Theorem, it is enough to show that, regardless of the choice of projector set $\{\hat{\Pi}_a^A\}$, $\mathcal{W}_{\{\hat{\Pi}_a^A\}} - \mathcal{W} = 0 \Rightarrow \overrightarrow{\mathcal{D}}_{SA} = 0$. Let assume that $\overrightarrow{\mathcal{D}}_{SA} \neq 0$. Then, there is at least a set $\{\hat{\Pi}_a^A\}$ such that $\mathcal{W}_{\{\hat{\Pi}_a^A\}} - \mathcal{W} \neq 0$. Two cases are then possible:

(i) There is a measurement outcome $\bar{a}$ such that $\hat{\rho}_{S|\bar{a}} \neq \sum_k r_k^{\bar{a}} |r_k\rangle \langle r_k|$ with $r_k^{\bar{a}} \geq r_{k+1}^{\bar{a}}$. Then

$$\mathcal{W}_{\{\Pi_a^A\}} - \mathcal{W} \geq p_{\bar{a}} \sum_{k,j} r_j^{\bar{a}} \epsilon_k \left(|\langle r_k| r_j^{\bar{a}} \rangle|^2 - \delta_{kj} \right) > 0, \tag{72}$$

given that $\sum_{k,j} r_j^{\bar{a}} \epsilon_k \left(|\langle r_k| r_j^{\bar{a}} \rangle|^2 - \delta_{kj} \right)$ is the ergotropy of $\hat{\rho}_{S|\bar{a}}$ relative to the Hamiltonian $\sum_k \epsilon_k |r_k\rangle \langle r_k|$, and is zero if and only if $\hat{\rho}_{S|\bar{a}} = \sum_k r_k^{\bar{a}} |r_k\rangle \langle r_k|$.

(ii) For every a $\rho_{S|a} = \sum_k r_k^a |r_k\rangle \langle r_k|$ with $r_k^a \geq r_{k+1}^a$. In this case $\mathcal{W}_{\{\Pi_a^A\}} - \mathcal{W} = 0$. However, as $\hat{\rho}_{SA}$ is such that $\overrightarrow{\mathcal{D}}_{SA} \neq 0$, it is always possible to identify another set $\{\hat{\Pi}_a'^A\}$ such that $\mathcal{W}_{\{\Pi_a'^A\}} - \mathcal{W} > 0$. In order to show how this is possible, we note that $\hat{\rho}_{SA}$ can be written as

$$\hat{\rho}_{SA} = \sum_{a,a'} \sum_{k,k'} C_{kk'}^{aa'} |r_k\rangle \langle r_{k'}|_S \otimes |a\rangle \left\langle a' \right|_A$$

with the condition $p_a C_{kk'}^{aa} = r_k^a \delta_{kk'}$. As $\overrightarrow{\mathcal{D}}_{SA} \neq 0$, there are two measurement outcomes $\bar{a}$ and $\bar{a}'$ such that $C_{kk'}^{\bar{a}\bar{a}'} \neq C_k^{\bar{a}\bar{a}'} \delta_{kk'}$. Should this be not true, we would have $\overrightarrow{\mathcal{D}}_{SA} = 0$, and thus a contradiction. Therefore, as $\overrightarrow{\mathcal{D}}_{SA} \neq 0$, the matrix ${}_A\langle \bar{a}| \hat{\rho}_{SA} |\bar{a}'\rangle_A$ cannot be diagonal in the basis $\{|r_k\rangle_S\}$ (here $|\bar{a}_A\rangle$ is the eigenstate of $\hat{\Pi}_a^A$ with eigenvalues $\bar{a}$). If $\bar{a} = \bar{a}'$, case (*ii*) cannot occur.

However, if $\bar{a} \neq \bar{a}'$, we can define the new set of projectors $\{\hat{\Pi}_a'^A\}$ with elements $\hat{\Pi}_{\bar{a}}'^A = (|\bar{a}\rangle + |\bar{a}'\rangle)(\langle \bar{a}| + \langle \bar{a}'|)/2$, $\hat{\Pi}_{\bar{a}'}'^A = (|\bar{a}\rangle - |\bar{a}'\rangle)(\langle \bar{a}| -$

$\langle\bar{a}'|)/2$ and $\hat{\Pi}'^A_a = \hat{\Pi}^A_a$ for $a \neq \bar{a}, \bar{a}'$. Then, the density matrix $\hat{\rho}'_{S|\bar{a}} = \mathrm{Tr}_A\{\hat{\Pi}'^A_{\bar{a}}\hat{\rho}_{SA}\}/p'_{\bar{a}}$ reads

$$\begin{aligned}\hat{\rho}'_{S|\bar{a}} = \frac{1}{2p'_{\bar{a}}}\Big[&\sum_k (p_{\bar{a}} r^{\bar{a}}_k + p_{\bar{a}'} r^{\bar{a}'}_k)\,|r_k\rangle\langle r_k|_S \\ &+ \left({}_A\langle\bar{a}|\,\hat{\rho}_{SA}\,|\bar{a}'\rangle_A + {}_A\langle\bar{a}'|\,\hat{\rho}_{SA}\,|\bar{a}\rangle_A\right)\Big],\end{aligned} \tag{73}$$

which shows that $\hat{\rho}'_{S|\bar{a}}$ is not diagonal in the basis $\{|r_k\rangle_S\}$. Therefore $\rho'_{S|\bar{a}} \neq \sum_k r'^{\bar{a}}_k |r_k\rangle\langle r_k|_S$ with $r'^{\bar{a}}_k \geq r'^{\bar{a}}_{k+1}$. So, proceeding in a similar way as for case (i), we conclude that

$$\mathcal{W}_{\{\Pi'^A_a\}} - \mathcal{W} > 0. \tag{74}$$

If ${}_A\langle\bar{a}|\,\hat{\rho}_{SA}\,|\bar{a}'\rangle_A + {}_A\langle\bar{a}'|\,\hat{\rho}_{SA}\,|\bar{a}\rangle_A = 0$, it is enough to consider $\hat{\rho}'_{S|\bar{a}'}$ instead of $\hat{\rho}'_{S|\bar{a}}$. ∎

Having proven Theorem 4.2.1, we can provide a justification of two important Corollaries

Corollary 4.A.2 *Under the premises of Theorem 4.2.1,* $\delta\mathcal{W} = 0 \nRightarrow \overleftarrow{\mathcal{D}}_{SA} = 0$.

Proof It is enough to consider the state

$$\hat{\rho}_{SA} = \sum_{k,a} q_{ak}\,|r_k\rangle\langle r_k|_S \otimes |\phi_a\rangle\langle\phi_a|_A\,, \tag{75}$$

where $\{|\phi_a\rangle_A\}$ is a non orthogonal set of states, such that we have $\overleftarrow{\mathcal{D}}_{SA} \neq 0$. If we choose q_{ak} such that $q_{ak} \geq q_{ak+1}$, we have $\mathcal{W}_{\{\hat{\Pi}^A_a\}} - \mathcal{W} = 0$ for any set $\{\hat{\Pi}^A_a\}$, as $\hat{\rho}_{S|a} = \sum_k r^a_k |r_k\rangle\langle r_k|_S$ with $r^a_k = \sum_{a'} q_{a'k}\,|\langle\phi_{a'}|\,a_A\rangle|^2/p_a \geq r^a_{k+1}$). ∎

Corollary 4.A.3 *Under the premises of Theorem 4.2.1, we have that* $\overleftarrow{\mathcal{D}}_{SA} = 0$ *or* $\overrightarrow{\mathcal{D}}_{SA} = 0 \nRightarrow \delta\mathcal{W} = 0$.

Proof We consider the state $\hat{\rho}_{SA} = \sum_k r_k \hat{\Pi}^S_k \otimes \hat{\Pi}^A_k$, where $\hat{\Pi}^A_k$ and $\hat{\Pi}^S_k$ are orthogonal projectors of rank one. Although such state has zero discord, the quantity $\mathcal{W}_{\{\Pi^A_k\}} - \mathcal{W}$ is positive since

$$\mathcal{W}_{\{\Pi^A_k\}} - \mathcal{W} = \sum_k r_k\epsilon_k - \epsilon_1 > 0. \tag{76}$$

Therefore, $\delta\mathcal{W} > 0$. ∎

We can now provide a proof of Theorem 4.2.2, which we state again for easiness of consultation.

Theorem 4.2.2 *For any system S and ancilla A prepared in a pure state $\hat{\rho}_{SA} = |\psi\rangle\langle\psi|_{SA}$ we have*

$$\delta\mathcal{W} = 0 \Leftrightarrow |\psi\rangle_{SA} \text{ is separable,} \tag{77}$$

and $\delta\mathcal{W} = \sum_k r_k \epsilon_k - \epsilon_1$, where r_k are the Schmidt coefficients of $|\psi\rangle_{SA}$ and ϵ_k are the eigenvalues of $\hat{H}_S$, ordered such that $r_k \geq r_{k+1}$ and $\epsilon_k \leq \epsilon_{k+1}$.

Proof We consider the pure state $\hat{\rho}_{SA} = |\psi_{SA}\rangle\langle\psi_{SA}|$ having the Schmidt decomposition $|\psi_{SA}\rangle = \sum_k \sqrt{r_k}\,|r_k\rangle_S \otimes |\phi_k\rangle_A$, with $r_k \geq r_{k+1}$. Then, we observe that choosing $\hat{\Pi}^A_a = |\phi_a\rangle\langle\phi_a|_A$ the work $\mathcal{W}_{\{\hat{\Pi}^A_a\}}$ is the biggest possible, since the final state of the protocol is always the ground state with energy ϵ_1. That implies the Eq. $\delta\mathcal{W} = \sum_k r_k \epsilon_k - \epsilon_1$. ∎

4.A.1 Analysis of the two-qubit case

We provide additional details on the analysis performed on the two-qubit case illustrated in the Chapter.

In what follows, with no loss of generality, we choose the system Hamiltonian $\hat{H}_S = -\hat{\sigma}_z$. We choose concurrence as the entanglement measure to be used in our analysis. For a bipartite qubit state, concurrence is defined as [71]

$$\mathcal{C} = \max[0, \lambda_1 - \sum_{j>1} \lambda_j], \tag{78}$$

where λ_k are the square roots of the eigenvalues of $\hat{\rho}\hat{\tilde{\rho}}$ with $\hat{\tilde{\rho}} = (\hat{\sigma}_y \otimes \hat{\sigma}_y)\hat{\rho}^*(\hat{\sigma}_y \otimes \hat{\sigma}_y)$, ordered so that $\lambda_k \geq \lambda_{k+1}$. Above, we have proven that the ergotropic gain of any state $\hat{\rho}_{SA}$ with concurrence $\mathcal{C}$ is larger than, or equal to

$$\delta\mathcal{W}_{\min}(\mathcal{C}) = 1 - \sqrt{1 - \mathcal{C}^2}. \tag{79}$$

The states locally equivalent to

$$\hat{\rho}_{SA} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & x & \mathcal{C}/2 & 0 \\ 0 & \mathcal{C}/2 & 1-x & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \tag{80}$$

with $x = (1 \pm \sqrt{1-\mathcal{C}^2})/2$, which have concurrence $\mathcal{C}$, are such that $\delta\mathcal{W} = \delta\mathcal{W}_{\min}(\mathcal{C})$. These states belong to the class parametrized as $p\left|\phi_+^\eta\right\rangle\left\langle\phi_+^\eta\right| + \frac{1-p}{2}(\left|01\right\rangle\left\langle 01\right| + \left|10\right\rangle\left\langle 10\right|)$ where $\left|\phi_+^\eta\right\rangle = \sqrt{\eta}\left|01\right\rangle + \sqrt{1-\eta}\left|10\right\rangle$. On the other hand, the states locally equivalent to

$$\hat{\rho}_{SA} = \begin{pmatrix} 1/2 & 0 & 0 & \mathcal{C}/2 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \mathcal{C}/2 & 0 & 0 & 1/2 \end{pmatrix}, \tag{81}$$

which also have concurrence $\mathcal{C}$, are such that $\delta\mathcal{W} = 1$, and thus embody the upper bound to the daemonic ergotropy at set value of concurrence.

In order to show this, we parameterize the projectors $\hat{\Pi}_1^A$ and $\hat{\Pi}_2^A$ that are needed to calculate the daemonic ergotropy in terms of the angles $\theta \in [0,\pi]$ and $\phi \in [0, 2\pi)$ such that

$$\Pi_1^A = \begin{pmatrix} \cos^2(\theta/2) & e^{-i\phi}\sin(\theta/2) \\ e^{i\phi}\sin(\theta/2) & \sin^2(\theta/2) \end{pmatrix}$$

and $\Pi_2^A = \mathbb{1} - \Pi_1^A$. An extensive numerical analysis of the distribution itself has shown that the states lying on the lower boundary belong to the class of so-called x-*states* of the form

$$\rho_{SA} = \begin{pmatrix} a & 0 & 0 & z \\ 0 & b & w & 0 \\ 0 & w & c & 0 \\ z & 0 & 0 & d \end{pmatrix}, \tag{82}$$

where a, b, c, d, w, z are positive numbers such that $bc \geq w^2$, $ad \geq z^2$. This class plays a key role in the characterisation of the states that maximize quantum correlations at set values of the purity of a given bipartite qubit state [72, 73, 74]. The ergotropy $\mathcal{W}$ for such class of states is

$$\mathcal{W} = \begin{cases} 0 & \text{for } a+b \geq \frac{1}{2}, \\ 2-4(a+b) & \text{otherwise.} \end{cases} \tag{83}$$

On the other hand, we have $\mathcal{W}_{\{\Pi_a^A\}} = 1 - 2(a+b) + (X_+ + X_-)/2$ with

$$X_\pm = \Big\{[2(a+b) - 1 \pm (1-2b-2c)\cos\theta]^2 + 4\left[we^{-i\phi} + ze^{i\phi}\right|^2 \sin^2\theta\Big\}^{\frac{1}{2}} . \tag{84}$$

The associated concurrence is $\mathcal{C} = 2\max\{0, z - \sqrt{bc}, w - \sqrt{ad}\}$. We make the ansatz that a state as in Eq. (80) with x real and positive, minimizes $\delta\mathcal{W}$ at a fixed value of $\mathcal{C}$. Then, from the positivity of the density matrix, x must satisfy the condition $\mathcal{C} \leq 2\sqrt{x(1-x)}$ with $x \in [0,1]$.

For such state, we have $\delta\mathcal{W} = 2 - 2x - \max\{0, 2-4x\}$. If we consider $x \geq 1/2$, then $\delta\mathcal{W} = 2 - 2x$, which is minimum when x is maximum, i.e. for $x = (1+\sqrt{1-\mathcal{C}^2})/2$. For $x \leq 1/2$ we have $\delta\mathcal{W} = 2x$, which is minimum when x is minimum, i.e. for $x = (1-\sqrt{1-\mathcal{C}^2})/2$. In both cases, $\delta\mathcal{W}$ takes the expression in Eq. (79).

In order to show that the class in Eq. (81) is such that $\delta\mathcal{W} = 1$, it is enough to observe that, for such state, $\mathcal{W} = 0$. In fact, we trivially have $\rho_S = \mathbf{1}/2$ and, by choosing for instance $\hat{\Pi}_1^A = |0\rangle\langle 0|_A$, we get pure post-measurement states, and thus $\mathcal{W}_{\{\hat{\Pi}_a^A\}} = 1$. Therefore $\delta\mathcal{W} = 1$ regardless of the value taken by $\mathcal{C}$.

Part III.

Applications to Specific Systems

5 LOCAL DISTURBANCE IN A QUANTUM ISING MODEL

In this Chapter, we study the out of equilibrium properties of a many-body system, with a particular emphasis on the thermodynamic work, when it is brought far from the equilibrium by a disturbance localized at its boundary.

We consider an exactly solvable system, namely, the Ising open chain in a transverse homogeneous field. The role of the disturbance is played by a defect in the field.

This model is a paradigmatic example in the field of the quantum phase transitions (QPT) [75], and a particular attention has been already paid to the study of the statistics of the work in this system [76, 77].

Furthermore, the model is formally equivalent to a Kitaev chain [78], which exhibits the existence of two Majorana zero modes in its non trivial topological phase. These modes are localized at the edges of the systems, which clarifies the importance of an analysis when the system is boundary-driven far from the equilibrium.

In Sec. 5.1 the model is introduced, and its static properties are discussed in terms of a fermionic representation. A spectral analysis is carried out in terms of fermionic modes. Among the delocalized modes, spatially localized modes can arise, and the condition and the nature of this effect are discussed in detail.

In Sec. 5.2, a study of the non equilibrium thermodynamics of the system is carried out. The effects of the local disturbance are studied in the out of equilibrium process generated by an abrupt change of the defect (*sudden quench*). We present a study of the statistics of the work, similar to those done in [76, 77]. We show how the thermodynamic quantities characterizing the process display a non analytic behavior at the absolute zero temperature.

In Sec. 5.3, the propagation of disturbances along the chain following the sudden quench, is characterized in terms of the transverse magnetization [C], and we show how the existence of the Majorana zero mode strongly influences the transient regime in the time evolution of the magnetization.

5.1 ISING MODEL IN A TRANSVERSE FIELD WITH DEFECT

A class of many body systems that is widely studied in condensed matter physics is the one composed by spins systems. Among these systems, the one dimensional chains formed by spin $\frac{1}{2}$, play a relevant role, also because their theorical study is relatively easy [79, 80]. From the technologic point of view, such systems could be adopted as channel for short distance quantum communications [81].

In that broad set of systems, when the mutual interactions have a short range, a reference model is given by the Hamiltonian

$$\hat{H}_{ss} = \sum_i \left\{ J_x \hat{S}^x_i \hat{S}^x_{i+1} + J_y \hat{S}^y_i \hat{S}^y_{i+1} + J_z \hat{S}^z_i \hat{S}^z_{i+1} \right\} \tag{85}$$

Here, the spin at the i^{th} site of the chain is described by the operator $\hat{\boldsymbol{S}}_i$. Physically, this kind of interaction can have a magnetic origin or can derive from an exchange interaction [82], and recently such models have been realized and studied in laboratory [83, 84]. For a closed chain $\hat{\boldsymbol{S}}_1 = \hat{\boldsymbol{S}}_{N+1}$, the sum in Eq. (85) goes from 1 to the total number of sites N, while for a open chain with free ends, the same sum goes from 1 to $N-1$.

From the Hamiltonian in Eq. (85) several models can be derived [85, 80, 79, 86], in particular the XY model originally studied by Lieb, Schultz and Mattis in [79], is obtained from Eq. (85) by putting $J_z = 0$.

The Ising Model (IM) [85] that we are going to consider, belongs to the same universality class of XY systems, and when a transverse homogeneous magnetic field is included, the IM becomes a paradigmatic example in the field of the quantum phase transitions (QPT) [75].

The IM in transverse field can be described by the Hamiltonian

$$\hat{H}_{Is} = J \sum_i \left\{ \hat{\sigma}_i^x \hat{\sigma}_{i+1}^x - h \hat{\sigma}_i^z \right\} ,$$

which is invariant under the "parity" transformation $\hat{\Pi} = e^{i\frac{\pi}{2}\sum_{i=1}^{N}(1-\hat{\sigma}_i^z)}$ (the system has a $\mathbb{Z}_2$ spin reflection symmetry [75]).

In the thermodynamic limit ($N \to \infty$), two quantum phases can be distinguished [75] depending on the value of the parameter h, here considered non negative.

If the field is strong enough $h \gg 1$, the spins tend to get the orientation imposed by the field, and the system is in a Paramagnetic Phase (PP) characterized by a non-degenerate ground state. As the field gets weak, and the critical value $h_c = 1$ is reached, the system becomes gapless (the energy gap between the continuum part of the spectrum and the ground state is closed), and a second order QPT takes place [75]. For values of h below h_c, the ground state is two-fold degenerate and the system displays long range order, as seen from the spin correlation functions [87, 88], and so there is a non zero spontanous magnetization (along x). In this Ordered Phase (OP), the two degenerate ground states have different parities, and a spontaneous breaking of the $\mathbb{Z}_2$ symmetry can occur. Technically, one or the other of the two states will be chosen the actual ground state by some infinitesimal external perturbation.

At the critical point $h = h_c$, the correlation length diverges as $|h - h_c|^{-\nu}$, and the excitation gap vanishes like $|h - h_c|^{z\nu}$, where the universal critical exponents are $z = \nu = 1$.

The out of equilibrium dynamics of the IM generated by a time dependent field h, was originally studied by Barouch, MacCoy et al. (for a XY model) [89, 90, 88, 91], and most recently by Calabrese et al. [92, 93, 94, 95]

For free ends boundary conditions, thanks to a Jordan-Wigner transformation [96], the spin system can be mapped into a non interacting fermionic gas, which can be identified with a Kitaev chain [78].

The phase diagram of this latter model has been studied in detail [97], and it is known to display a topologically non-trivial phase, and a trivial one, that are mapped into the PP and the OP of the IM, respectively [98].

Because of this relation with the Kitaev chain, we focus on a Ising open chain subject to an external disturbance localized on one of the two edges of the chain.

We consider a defect in the transverse field h, so that the system is described by the Hamiltonian

$$\hat{H}_{\mu} = -\mu h \hat{\sigma}_1^z - h \sum_{n=2}^{N} \hat{\sigma}_n^z + \sum_{n=1}^{N-1} \hat{\sigma}_n^x \hat{\sigma}_{n+1}^x \tag{86}$$

where μ is used to parameterize the field defect, and we have taken the exchange constant J as our energy unit, $J = 1$.

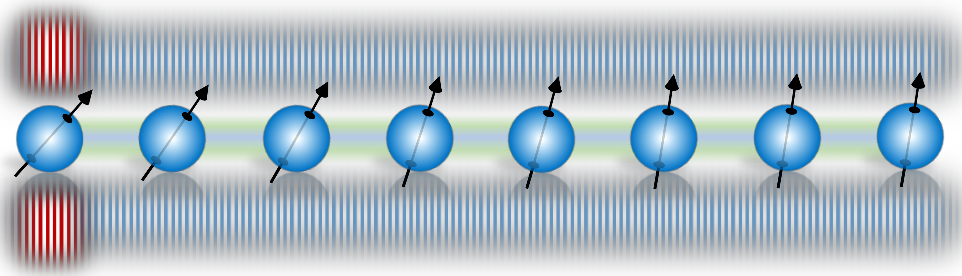

Figure 5.1.1.: The picture summarizes the model described by the Hamiltonian in Eq. (86). The one-dimensional chain of N spins 1/2 with nearest-neighbor "Ising" interactions, is subject to a homogeneous transverse magnetic field. This field can be manipulated locally at one edge of the chain.

5.1.1 Energy Spectrum and Spatial Localization

The system with Hamiltonian given in Eq. (86) is studied in the Jordan-Wigner representation [96].

As shown in the App. 5.A, the fermionic Hamiltonian can be recast in the form

$$\begin{aligned}\hat{H}_\mu &= \sum_k \Lambda_k \left(\hat{\eta}_k^\dagger \hat{\eta}_k - \frac{1}{2}\right) \\ &= \sum_{\kappa\in\mathcal{K}} \Lambda_\kappa \left(\hat{\eta}_\kappa^\dagger \hat{\eta}_\kappa - \frac{1}{2}\right) + \sum_{i=1,2} \chi_i \Lambda_{(i)} \left(\hat{\eta}_{(i)}^\dagger \hat{\eta}_{(i)} - \frac{1}{2}\right)\end{aligned} \tag{87}$$

where the η operators satisfy the canonical anticommutation relations $\{\hat{\eta}_k, \hat{\eta}_q\} = 0$, $\{\hat{\eta}_k^\dagger, \hat{\eta}_q\} = \delta_{kq}$.

In this representation, the energy eigen-states are identified by the set of the occupation numbers $\{n_k\}_k$ of the quasi-particles η [99], and the eigen-energies are $E(\{n_k\}) = \sum_k \left(n_k - \frac{1}{2}\right)\Lambda_k$. All the frequencies Λ_k are non-negative, and so the energy of the ground state is given by $E_{GS} = -\sum_k \Lambda_k/2$.

In Eq. (87), the index κ does not refer to linear momentum because the system is not translationally invariant, but it runs over a quasi-continuous band of delocalized modes having energy $\Lambda_\kappa = \Lambda(\theta_\kappa) = 2\sqrt{1+h^2-2h\cos(\theta_\kappa)}$. Two *discrete* localized modes can appear depending on the value of the field h and of the defect parameter μ.

These two modes, labeled with (1) and (2), in the thermodynamic limit have frequencies $\Lambda_{(1)} = 0$ and $\Lambda_{(2)} = 2|\mu|\sqrt{\frac{1+(\mu^2-1)h^2}{\mu^2-1}}$, and exist if $(h,\mu) \in \mathcal{R}_1$ and if $(h,\mu) \in \mathcal{R}_2$, respectively (see Fig. (5.1.2)). The regions $\mathcal{R}_{1,2}$ are defined in Eq. (120).

If $\mu = 0$, the system is symmetric with respect to an arbitrary rotation of the first spin around the x axis, generated by $\hat{\sigma}_1^x$. Then, given an eigenstate of $\hat{H}_0$, the state of the first spin is factorized from the rest of the chain, and it is one of the two eigenstates of $\hat{\sigma}_1^x$.

In this special case, the two modes (1) and (2) have frequencies equal to zero, $\Lambda_{(1)} = \Lambda_{(2)} = 0$, also for finite N (as discussed in App. 5.A).

If all the single particle energies are positive, the ground state $|GS\rangle$ of the system is non degenerate, and it is represented by the vacuum state defined by $\hat{\eta}_k|\tilde{0}\rangle = 0$ for every k.

If $\mu = 0$, or if $h < 1$ (in the thermodynamic limit), the ground state is two-fold degenerate because there is a localized mode having zero frequency.

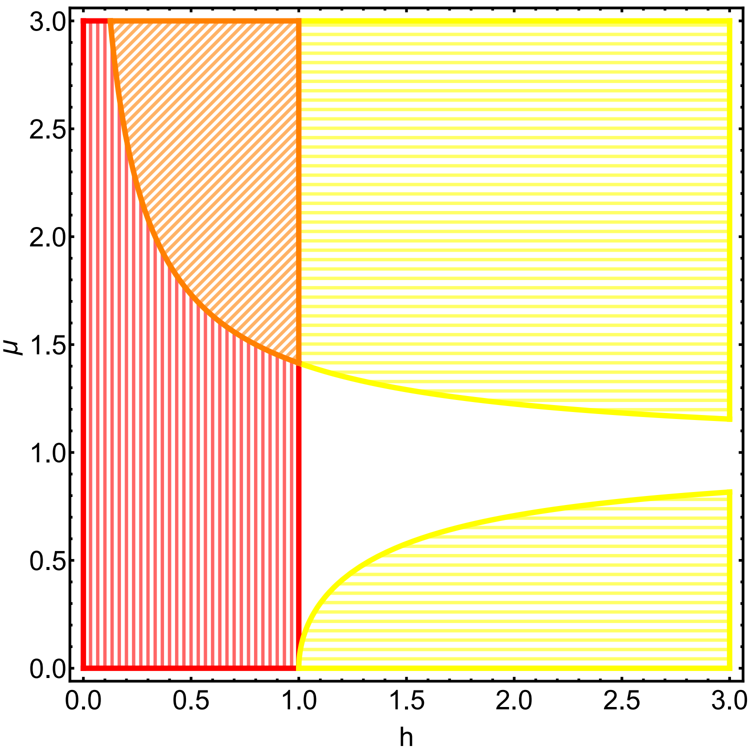

Figure 5.1.2.: Phase diagram showing the presence of the localized modes $\Lambda_{(i)}$ $(i = 1, 2)$ in the h, μ plane. The red region (vertical lines), $\mathcal{R}_1$, features the presence of the mode with frequency $\Lambda_{(1)}$. The yellow region (horizontal lines) $\mathcal{R}_2$, instead, features the presence of mode (2), either below or above the band in the two subregions with μ smaller or larger than $\mu = 1$, respectively. Both of the localized modes are present in the orange region (oblique lines), corresponding to the intersection of $\mathcal{R}_1$ and $\mathcal{R}_2$. Finally, only delocalized modes are present in the white region.

Explicitly, for $N \to \infty$, the mode (1) has a topological origin. If the transverse field is homogeneous $\mu = 1$, then the mode (1) can be identified with the Majorana zero mode discussed by Kitaev in [78]. It is topologically protected [78] and so it survives during a continuous change of the Hamiltonian until the system stays gapped. Since the gap is closed at $h = h_c$, the Majorana zero mode of H_1 survives for every inhomogeneity μ if $h < 1$, and the "wave" functions $\psi_n^{(1)}$ and $\phi_n^{(1)}$ given in Eq. (129), stay localized on the last and the first site of the chain, respectively.

Conversely the mode (2) is generated by the inhomogeneity, that heuristically speaking tends to decouple the first spin from the rest of the chain. This mode stays localized near the first site, as it is shown by the wave functions $\psi_n^{(2)}$ and $\phi_n^{(2)}$ given in Eq. (131). The frequency $\Lambda_{(2)}$ is zero only at $\mu = 0$, and since $\Lambda_{(2)}$ is non negative, it needs to be a non analytic function of the parameters h and μ on the line defined by $\mu = 0$.

This non regular behaviour can be observed in some physical properties of the system.

An illustrative example is given by the transverse magnetization on the first site $\langle \hat{S}_1^z \rangle$ calculated with respect to the ground state $|GS\rangle$. For a finite N, it is

$$\lim_{\mu \to 0^\pm} \langle \hat{S}_1^z \rangle = \pm \frac{1}{2h} \sqrt{\frac{h^2 - 1}{1 - h^{-2N}}} \tag{88}$$

and in the themodynamic limit

$$\lim_{\mu \to 0^\pm} \langle \hat{S}_1^z \rangle = \pm \frac{\sqrt{h^2 - 1}}{2h} \Theta(h - 1) \tag{89}$$

where $\Theta(x)$ is the step function, defined to be one if $x > 0$, or zero elsewhere.

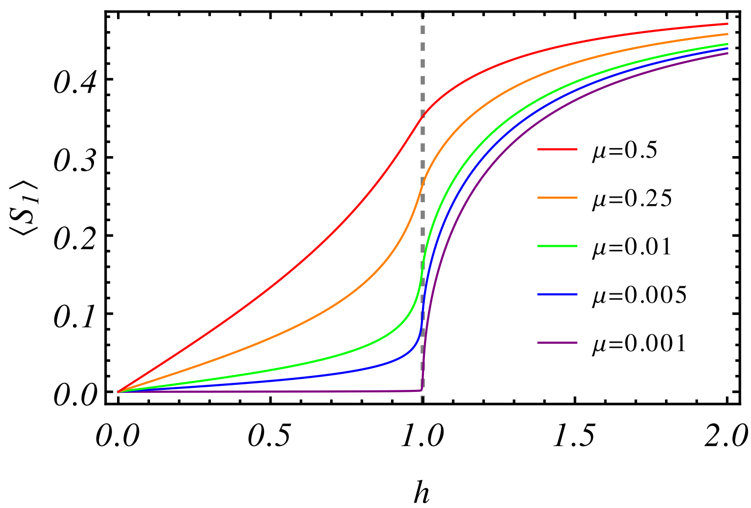

Figure 5.1.3.: Transverse magnetization of the defect spin as a function of the magnetic field for various defect's strength μ, for $N = 1000$.

The longitudinal magnetization $\langle \hat{S}_1^x \rangle$ could be non zero only if the ground state is degenerate. In the thermodynamic limit this occurs in the ordered phase ($h < 1$), and if $\mu \neq 0$, we have [100] $m_1^x = \left|\langle \hat{S}_1^x \rangle\right| = \frac{1}{2}\Theta(1-h)\phi_1^{(1)}$, and so

$$m_1^x = \frac{1}{2}\frac{\sqrt{1-h^2}}{\sqrt{1+(\mu^2-1)h^2}}\Theta(1-h) \tag{90}$$

One can understand qualitatively this behaviour, by thinking that when the parameters μ and h cross the line $\mu = 0$, the magnetic field in the first site reverses its direction. Then, though the first spin is in an eigen-state of $\hat{S}_1^x$ when μ is exactly equal to zero, such state is "unstable", even because a little perturbation on the defect could generate a non zero transverse magnetization m_1^x, given by Eq. (89). The fact that this happens only for $h > 1$ means that the dominant spin-spin interaction for $h < 1$ tends to forbid a non zero transverse magnetization in this region, and it could be attributed to the "topological properties" of the ordered phase.

5.2 THERMODYNAMICS

The thermodynamics of the model at thermal equilibrium in the Gibbs state ρ_G can be characterized by the Helmholtz free energy $F = -k_B T/lnZ$ where Z is the partition function

$$Z = 2^N \prod_{k=1}^{N} \cosh\left(\frac{\beta\Lambda_k}{2}\right)$$

In the fermionic representation, the transverse field plays the role of a chemical potential, and the state is described by a grand canonical ensemble.

For large N, the Helmholtz free energy reads

$$\begin{aligned} F &= -\frac{1}{\beta}\sum_{\kappa\in\mathcal{K}} \ln\left[2\cosh\left(\frac{\beta\Lambda(\theta_\kappa^0)}{2}\right)\right] - 2h\sum_{\kappa\in\mathcal{K}} \tanh\left(\frac{\beta\Lambda(\theta_\kappa^0)}{2}\right)\frac{\sin(\theta_\kappa^0)}{\Lambda(\theta_\kappa^0)}(\theta_\kappa - \theta_\kappa^0) \\ &\quad -\frac{1}{\beta}\sum_i \chi_i \ln\left[2\cosh\left(\frac{\beta\Lambda_{(i)}}{2}\right)\right] + \mathcal{O}(1/N) \end{aligned} \tag{91}$$

where θ_κ^0 is a point in the interval $I_\kappa = [\frac{(\kappa-1)\pi}{N}, \frac{\kappa\pi}{N}]$, and θ_κ are given in Eq. (118). The contribution of order N to the free energy is

$$F = -\frac{1}{\beta}\frac{N}{\pi}\int_0^\pi \ln\left(2\cosh\left(\frac{\beta\Lambda(\theta)}{2}\right)\right)d\theta + \mathcal{O}(1)$$

and so at a macroscopic level, the thermodynamics is substantially the same as for the Ising model in a homogenous transverse field studied in [87, 75]. As $T \to 0$, the free energy F tends to the ground state energy E_{GS}, and the system undergoes a QPT at $h = 1$ since

$$\lim_{N\to\infty}\frac{E_{GS}}{N} = -\frac{2(1+h)}{\pi}E\left(\frac{\pi}{2}, \frac{4h}{(1+h)^2}\right) \tag{92}$$

where $E(\phi, x)$ is the elliptic integral of the second kind, and it is non analytic at $h = 1$.

So the effects of the local disturbance on the thermodynamic behavior tend to be covered at a macroscopic level. They can be studied by considering the out of equilibrium thermodynamics of a local change of the Hamiltonian, that is referred to as local quench [76].

5.2.1 Local Quench

We assume that the system is initially prepared in the thermal Gibbs state $\hat{\rho}_G[\mu, T]$, and we perform a local sudden quench on one edge of the system, achieved by the instantaneous change of the defect parameter from μ to $\mu + \Delta\mu$, so that $\hat{H}_i = \hat{H}_\mu$ and $\hat{H}_f = \hat{H}_{\mu+\Delta\mu}$.

Though the disturbance is local, so that $\hat{H}_f - \hat{H}_i = -\Delta\mu h \hat{\sigma}_1^z$, the final and the initial Hamiltonian are non-compatible osservables, and $[\hat{H}_f, \hat{H}_i]$ is a non local operator. Then, the statistics of the work cannot be obtained only from the local properties of the system, as it is evident from Eq. (19).

Anyway, the characteristic function of the work can be determined by using a local probe made by a two level system. Initially the state of the probe is assumed to be uncorrelated with that of the spin chain, so that total state of the two systems is $\hat{\rho}_{tot}(0) = \hat{\rho}_{pr}(0) \otimes \hat{\rho}_G[\mu, T]$. The free evolution of the probe will be generated by the Hamiltonian $\hat{H}_{pr} = \omega_e |e\rangle \langle e|$, where $|e\rangle$ is its excited state, and the energy of the ground state is chosen as the energy reference point. Then, if the interaction between the two systems is described by $\hat{H}_{int} = -\epsilon |e\rangle \langle e| \otimes \hat{\sigma}_1^z$, and if the evolution of the total system is unitary, the spin chain induces a pure dephasing on the state of the probe [101], and the coherence of the probe can be recast in form

$$\langle e| \hat{\rho}_{pr}(t) |g\rangle = e^{-i\omega_e t}\chi^*(t) \tag{93}$$

where $\chi(u)$ is the work characteristic function when $\Delta\mu = \epsilon/h$.

The difference of free energy ΔF can be written as $\Delta F = F_1(\mu + \Delta\mu) - F_1(\mu)$, where $F_1(\mu)$ is the contribution of order one to the free energy, up to a constant that does not depend on μ. In the thermodynamic limit, we have

$$\begin{aligned} F_1(\mu) \quad = \quad & -\frac{2h}{\pi}\int_0^\pi \tanh\left(\frac{\beta\Lambda(\theta)}{2}\right)\frac{\sin(\theta)}{\Lambda(\theta)}\left(\arctan\mathcal{F}(\theta) + n(\theta)\pi\right)d\theta \\ & +\frac{1}{\beta}\left(\chi_1 + \chi_{2a}\right)\ln\left[2\cosh\left(\beta\left|h-1\right|\right)\right] + \frac{1}{\beta}\chi_{2b}\ln\left[2\cosh\left(\beta(1+h)\right)\right] \\ & -\frac{1}{\beta}\sum_i \chi_i \ln\left[2\cosh\left(\frac{\beta\Lambda_{(i)}}{2}\right)\right] \end{aligned}$$

where $\mathcal{F}(\theta)$ is defined in Eq. (116), and $n(\theta)$ is

$$n(\theta) = -\chi_1(1-\chi_{2b}) - \chi_{2a} - \Theta(\overline{\theta}-\theta)\chi_1\chi_2 - \Theta(\theta-\overline{\theta})(1-\chi_1)(1-\chi_2)$$

The average work is related to the magnetization on the first site by

$$\langle w\rangle = -\Delta\mu h \langle\hat{\sigma}_1^z\rangle_i$$

and it can be also expressed in terms of the variation of the free energy as

$$\langle w\rangle = \Delta\mu\frac{\partial F(\mu)}{\partial\mu}$$

In the thermodynamic limit

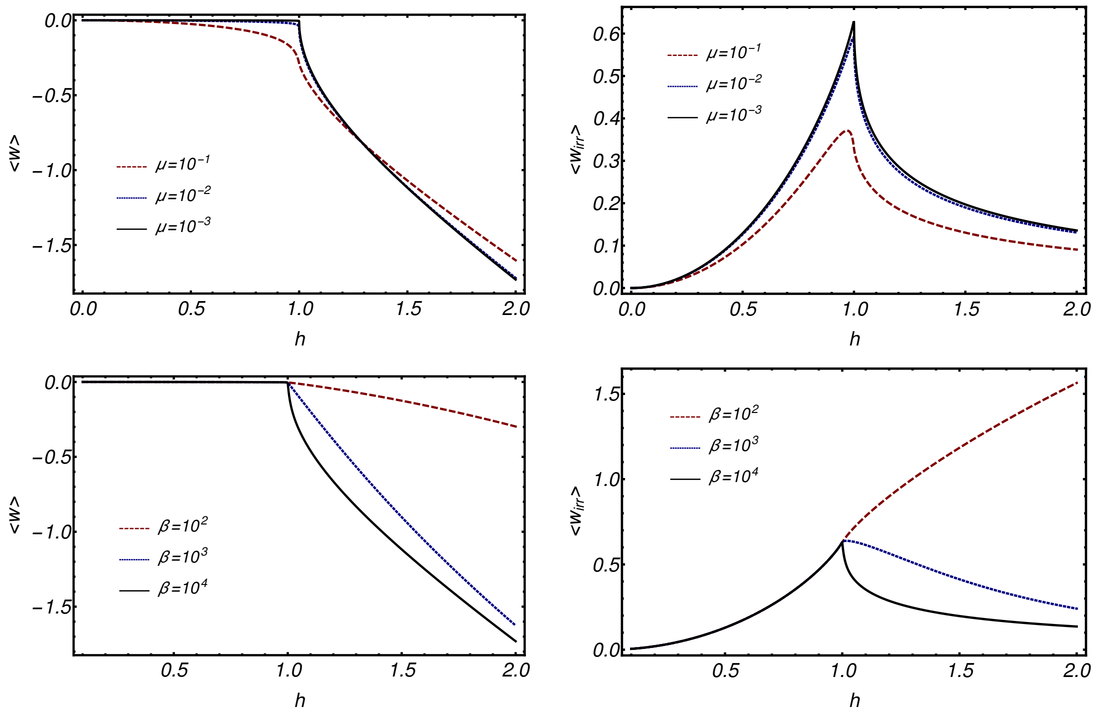

Figure 5.2.1.: (Color online): Work and irreversible work for the local quench $H_\mu \to H_1$. In the top panels we focus on the case of the absolute zero temperature limit. As $\mu \to 0$, the two quantities become non derivable at the point $h = 1$. In the bottom panels we put $\mu = 10^{-3}$, and we show how the quantities approach to the black line in the top panels, by lowering the temperature.

$$\begin{aligned} \frac{\partial F(\mu)}{\partial \mu} &= -\frac{4\mu h^2}{\pi}\int_0^\pi \frac{\sin^2(\theta)}{\left(1+h^2(\mu^2-1)^2+2h(\mu^2-1)\cos(\theta)\right)\Lambda(\theta)} \\ &\quad \times \tanh\left(\frac{\beta\Lambda(\theta)}{2}\right)d\theta + 2\chi_2\mu\frac{1-h^2(\mu^2-1)^2}{(\mu^2-1)^2\Lambda_{(2)}}\tanh\left(\frac{\beta\Lambda_{(2)}}{2}\right) \end{aligned} \tag{94}$$

and so only the mode (2) gives a substantial contribution, since the edge mode (1) has zero frequency.

The second moment of the work is $\langle w^2\rangle = (\Delta\mu h)^2$, and the third moment is $\langle w^3\rangle = (\Delta\mu h)^2\left(\langle w\rangle - 2\langle\sigma_1^x\sigma_2^x\rangle_i\right)$.

It is interesting to consider the limit $T \to 0$. For a fixed $\mu > 0$, the work $\langle w\rangle$ and the difference in free energy ΔF are non analytic at $h = 1$[1], and so is the

1 The third derivative with respect to h is non continuous in h at $h = 1$

irreversible work $\langle w_{irr}\rangle$. We note that $\langle w_{irr}\rangle$ shows at least one maximum in the interval $[0,\infty)$, because it is zero at the boundary of this interval.

As $\mu \to 0$, the derivative of the work with respect to h tends to be non continuous at $h = 1$, as can be seen from the magnetization expression in Eq. (89). In the limit $\mu \to 0^{\pm}$, the work is zero if $h < 1$, and, as $h \to 1^{+}$, it goes to zero like $\langle w\rangle \sim \mp\Delta\mu\sqrt{2}\sqrt{h-1}$.

The difference of free energy ΔF, and also the irreversible work $\langle w_{irr}\rangle$, have a non trivial dependence on $\Delta\mu$. In particular, if we turn off the defect by performing the quench $\Delta\mu = 1-\mu$, we have

$$\lim_{\mu\to 0^{+}} \langle w_{irr}\rangle = \frac{2h}{\pi}\int_0^{\pi} \frac{\sin(\theta)}{\Lambda(\theta)} \arctan\left(\frac{h\sin(\theta)}{1-h\cos(\theta)}\right) d\theta \tag{95}$$

and the irreversible work has a maximum point at $h = 1$, as can be seen from Fig. 5.2.1 (top panels).

In the limit $\mu \to 0^{\pm}$, as $h \to 1$, we have $\Delta F \sim (-2 + (h-1)\ln|h-1|)/\pi$ and

$$\langle w_{irr}\rangle \sim \frac{2}{\pi} + \begin{cases} \frac{1}{\pi}(1-h)\ln(1-h) & \text{if} \quad h\to 1^{-} \\ \mp\sqrt{2}\sqrt{h-1} & \text{if} \quad h\to 1^{+} \end{cases} \tag{96}$$

For finite N, the characteristic function of the work can be calculated by using a representation in terms of fermionic coherent states [102], and it reads

$$\chi(u) = \det\Big((U^T + V^T)(U + e^{iu\Lambda^{(f)}}V)\Big)\, e^{iu\left(E_{GS}^{(f)}-E_{GS}^{(i)}\right)} \tag{97}$$

where the matrices U and V are given in Eq. (138), and $\Lambda^{(f)}$ is the diagonal matrix having diagonal elements $\Lambda_k^{(f)}$. From Eq. (97), it follows that the expression for the irreversible work is given by

$$\langle w_{irr}\rangle = E_{GS}^{(i)} - E_{GS}^{(f)} - i\chi^{(1)}(0) = \mathrm{Tr}\left\{(U^T+V^T)\Lambda^{(f)}V\right\} \tag{98}$$

In going out from the limit $T \to 0$, we need to pay a particular attention, because of the thermal fluctuations. We focus on the limiting case $|\mu| \ll 1$. The work performed is

$$\langle w\rangle = \Delta\mu\Theta(h-1)\tanh\left(\frac{\beta\Lambda_{(2)}}{2}\right)(1-h^2)\frac{2\mu}{\Lambda_{(2)}} + \mathcal{O}(\mu)$$

At high temperatures ($\beta|\mu| \ll 1$), the work is a $\mathcal{O}(\mu)$ function, since $\tanh(x) = \mathcal{O}(x)$ as $x \to 0$.

Instead, if the temperature is low enough ($\beta|\mu| \gg 1$) so that $\tanh\left(\frac{\beta\Lambda_{(2)}}{2}\right) \simeq 1 - 2e^{-\beta\Lambda_{(2)}}$, we have

$$\langle w\rangle \simeq -\frac{\mu}{|\mu|}\Delta\mu\Theta(h-1)\left(1-2e^{-\beta\Lambda_{(2)}}\right)\sqrt{h^2-1} + \mathcal{O}(\mu)$$

Then, up to terms that go to zero as $\mathcal{O}(\mu)$ when $\mu \to 0$, in the paramagnetic region, the system responds as a single $1/2$ spin with Larmor precession frequency $\Lambda_{(2)}$.

The behaviors of the work and of the irreversible work approaching to the limit $T \to 0$ are shown in the Fig. 5.2.1 (bottom panels).

5.3 DISTURBANCE PROPAGATION

In a short range interacting many body systems, it is expected that a finite maximum speed exists for the propagation of information within the system [103].

In particular, a recent work by Smacchia and Silva [104] discusses the propagation of magnetization after a local time dependent quench in the quantum Ising model.

The quench can be seen as a source of quasi-particles, that can carry magnetization and correlations [92, 104].

We study the dynamics following the sudden removal of the defect at the boundary, in a chain of finite size. The aim is to discuss how a local perturbation propagates in the system and, in particular, how the dynamics is affected by the localized mode (1), that is identified with the Majorana zero mode in the thermodynamic limit.

To this end, we assume the system to be initially prepared in the ground state $|GS\rangle_0$ of $\hat{H}_0$ (with $\mu = 0$).

At $t = 0$ the defect is suddenly removed ($\mu = 1$ for $t \geq 0$), so that the system's subsequent evolution is generated by the homogeneous Ising Hamiltonian $\hat{H}_1$, whose ground state we denote $|GS\rangle_1$.

The spatial structure of the initial state $|GS\rangle_0$ differs from that of $|GS\rangle_1$ near the first site only, as found in the magnetization contrast $\delta m_i = \langle \hat{S}_i^z \rangle_{GS_1} - \langle \hat{S}_i^z \rangle_{GS_0}$.

The magnetization contrast δm_i quantifies how much the magnetization of the ground state $|GS\rangle_1$ (the one of the Hamiltonian $\hat{H}_1$ that rules the dynamics) is perturbated by the local defect in the field, and it decays exponentially with the distance from the defect, $\delta m_i = \delta m_1 \exp(-(i-1)/\xi)$, with a short localization length ξ, see App. 5.C.

Once the defect is removed, the local magnetization peak travels through the chain, starting near site $i = 1$ at $t = 0$.

Two different scenarios occur, depending on the value of the transverse field h. For $h > 1$, after the quench the system only supports delocalized fermion eigen-modes (white region in Fig. 5.1.2). These will be shown to give rise to a purely ballistic propagation of the magnetization peak. In the ordered phase $0 < h < 1$, on the other hand, H_1 enjoys the localized mode with energy Λ_1, residing on the edge of the system, and substantially overlapping with the initial localized state $|GS\rangle_0$. A pinning of the excitation near the first site occurs in this case, due to the interplay of the otherwise ballistic propagation with the localized nature of the Majorana mode, and giving rise to temporal oscillations of the local magnetization.

In order to characterize the propagation of the magnetic perturbation along the chain, we consider the mean square magnetization center and its velocity, defined as

$$R^2(t) = \sum_{i=1}^{N} \delta m_i(t)(i-1)^2 \tag{99}$$

$$v(t) = \frac{d}{dt}\sqrt{|R^2(t) - R^2(0)|}. \tag{100}$$

where $\delta m_i(t) = \langle \hat{S}_i^z \rangle_{GS_1} - \langle \hat{S}_i^z(t) \rangle_{GS_0}$ is the time-dependent version of the magnetization contrast introduced above. Analogous variables have been adopted and experimentally measured in Ref. [105].

Using the diagonal form of H_1, one can show that

$$
\begin{aligned}
R^2(t) &= \sum_{k_1,k_2} A_{k_1\,k_2} \cos\left((\Lambda_{k_1} - \Lambda_{k_2})t\right) \\
&+ \sum_{k_1,k_2} B_{k_1\,k_2} \cos\left((\Lambda_{k_1} + \Lambda_{k_2})t\right)
\end{aligned}
$$

where the summations are performed over the eigenmodes of the final Hamiltonian H_1, including both the delocalized fermion modes κ, and, if $h < 1$, the

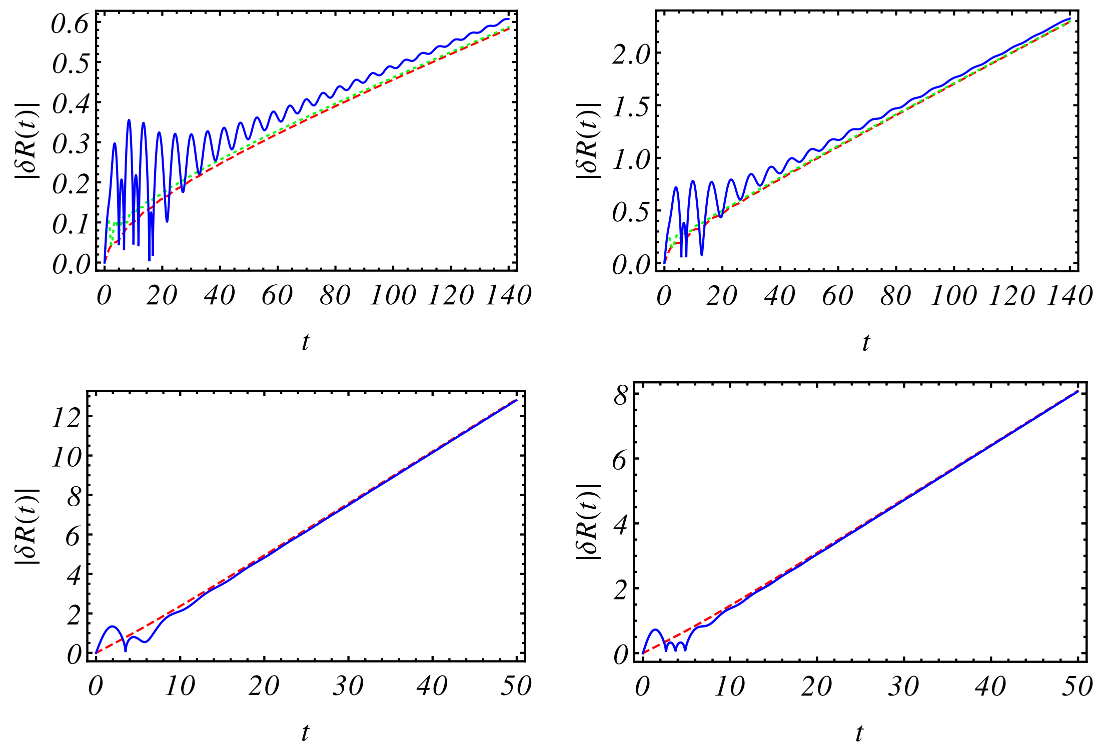

Figure 5.3.1.: (Color online): Detachment of the magnetization center from its initial position, $\delta R(t) = \sqrt{|R^2(t) - R^2(0)|}$, for (top left to bottom right) $h = 0.4, 0.6, 1.2, 1.6$, with $N = 100$. Solid blue lines are drawn by using the full expression for $R(t)$, whereas dashed red lines contain the rotating (A) contributions only. The dashed green lines are obtained from the blue ones by artificially excluding the contribution of the Majorana zero mode, in order to better highlight its role.

localized edge mode (1). The explicit form of the matrices A and B are given in App. 5.C; what is important here is that they give two different types of contribution to the propagating magnetization center: a rotating term, (A), and a counter-rotating one, (B).

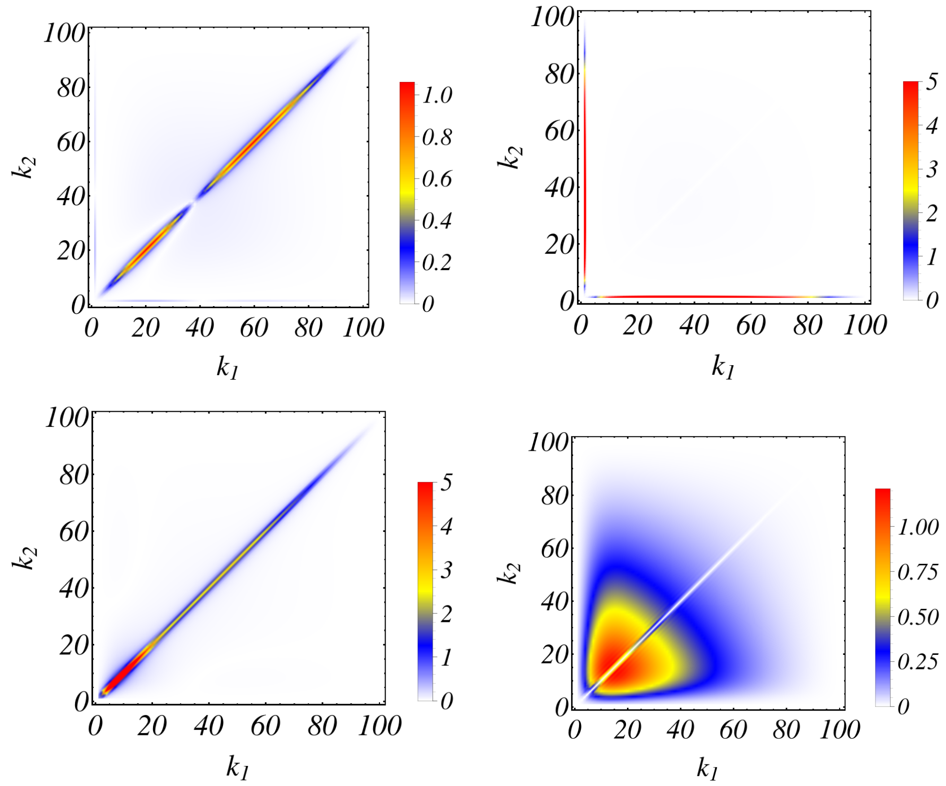

Figure 5.3.2.: (Color online): Elements of the matrices A (left panels) and B (right ones) for $h = 0.4$ (top) and $h = 1.4$ (bottom). The plots are made for $N = 100$.

In the thermodynamic limit, the asymptotic behavior of $R(t)$ is determined by the rotating terms with lower frequencies, as the B-contribution becomes negligible at long times due to their fast oscillations.

This is clearly seen in Fig. 5.3.1, where we show $\delta R(t) = \sqrt{|R^2(t) - R^2(0)|}$ for different values of the magnetic field h. In the plots, the solid blue curves giving $\delta R(t)$ are compared to the behaviors obtained by artificially keeping the A-contribution only.

This is done to better emphasize that B-terms only contribute to the transient oscillations, after which the propagation tends to be ballistic, and com-

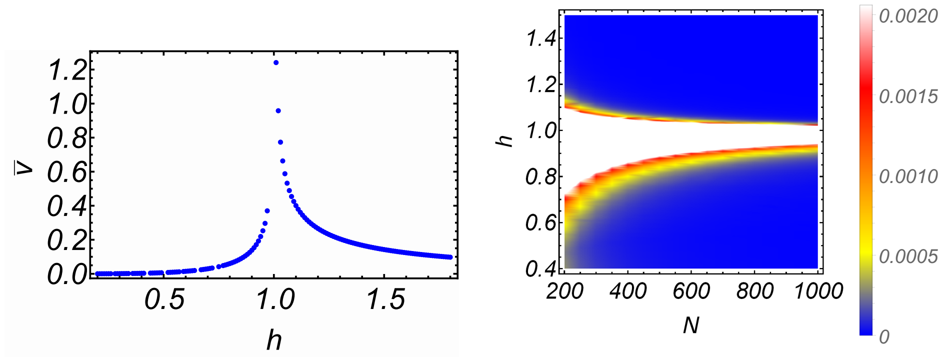

Figure 5.3.3.: (Color online): Left: Average asymptotic speed $\bar{v}$, taken in the long time limit (but before the occurrence of finite size revivals) as a mean over residual long time oscillations, for $N = 800$. Right: Scaling with the system size N and with the external field h of the amplitude of the long time oscillations displayed by the propagation speed $v(t)$ around the average $\bar{v}$. In the white region the limiting speed is not well defined because of the persistence of its oscillations

pletely accounted for by the lower frequencies terms, and the long-time speed is $\bar{v} \approx \sqrt{\sum_\kappa \frac{A_{\kappa\,\kappa+1}}{2} \left(\Lambda_\kappa - \Lambda_{\kappa+1}\right)^2}$.

Furthermore, by analyzing the matrix A as displayed in Fig. 5.3.2, we see that the main contribution comes from the entries close to the diagonal, so that this gives a very good approximation for the average propagation velocity in the disordered region, while it fails near the critical point $h = 1$, since the correlation length tends to be of the order of the size of the system, and $\delta R(t)$ and $v(t)$ keep oscillating even at long times, see Fig. 5.3.3. It also fails in the ordered region, because of the presence of the Majorana mode, coming into play via the counter rotating terms, see the matrix B in Fig. 5.3.2: the B contributions are basically irrelevant for $h > 1$, while their presence induces strong transient oscillations if $h < 1$, whose amplitude increases as $h \to 1^-$, see top panels in Fig. 5.3.1.

5.4 SUMMARY AND CONCLUSIONS

In this Chapter, we have studied a quantum Ising chain in a transverse homogeneous field, which is a paradigmatic example in the QPT field. The model is also intimaly related to the Kitaev chain, which shows Majorana zero modes localized at its boundary. For this reason, we consider the possibility to have an additional field, localized at one edge of the chain, producing a local defect in the transverse field. The defect strenght can be varied, generating a process that brings the system out of the equilibrium. The non equilibrium thermodynamics of this process is characterized in terms of the work done, investigating the role played by the QPT. Specifically, the work, the free energy difference and the irreversible work are studied when the system is initially prepared in a Gibbs state at a finite temperature, and in the limit of the absolute zero. In such limit, these thermodynamic quantities display a non analytical behavior at the critical point. The behavior of the work and the irreversible work changes substantially as the initial defect is such that the field at the edge is zero. The analysis has been carried on, considering the propagation of local magnetic excitation occurring when the defect is switched off. We have found that, though the propagation is ballistic, the magnetization could display some oscillations because of an involvement of the Majorana zero mode.

APPENDICES

5.A QUANTUM ISING MODEL: DIAGONALIZATION IN PRESENCE OF A DEFECT IN THE TRANSVERSE FIELD

The Ising model in a homogeneous transverse field, with a field inhomogeneity at one edge is characterized by the Hamiltonian

$$\hat{H}_\mu = -\mu h \hat{\sigma}_1^z - h \sum_{n=2}^{N} \hat{\sigma}_n^z + \sum_{n=1}^{N-1} \hat{\sigma}_n^x \hat{\sigma}_{n+1}^x \tag{101}$$

The operators $\hat{\sigma}_n^\alpha$ ($\alpha = x, y, z$) are the usual Pauli spin operator on site n, and $h > 0$.

In order to diagonalize the Hamiltonian in eq. 101, we work in the representation defined by the non-local Jordan-Wigner (J-W) transformation

$$\hat{c}_n^\dagger = \left(\prod_{j=1}^{n-1} \hat{\sigma}_j^z \right) \hat{\sigma}_n^- \tag{102}$$

where $\hat{\sigma}_j^\pm = (\hat{\sigma}_j^x \pm i \hat{\sigma}_j^y)/2$ are the raising and lowering spin operator, and the operators c act on a Fock space, and they satisfie the canonical anticommutation relations $\{c_n, c_m^\dagger\} = \delta_{n,m}$ and $\{c_n, c_m\} = 0$. The transformation in Eq. (102) fermionizes Eq. 101 into

$$\hat{H} = \sum_{i\,j} \left(\hat{c}_i^\dagger A_{i\,j} \hat{c}_j + \frac{1}{2} \left(\hat{c}_i^\dagger B_{i\,j} \hat{c}_j^\dagger + h.c. \right) \right) - Nh - (\mu - 1)h \tag{103}$$

where A and B are tridiagonal symmetric and anti-symmetric matrices respectively, whose elements are given by $A_{i\,j} = 2h(1 + \delta_{i1}(\mu - 1))\delta_{ij} + \delta_{i\,j+1} + \delta_{i+1\,j}$ and $B_{i\,j} = -\delta_{i\,j+1} + \delta_{i+1\,j}$. Since the Hamiltonian in Eq. 103 is a quadratic form in the creation and annihilation operators, it can be diagonalized by means of a Bogoliubov transformation:

$$\hat{c}_i = \sum_k u_{ik} \hat{\eta}_k + v_{ik} \hat{\eta}_k^\dagger \tag{104}$$

with the conditions $\sum_k u_{ik}u_{jk} + v_{ik}v_{jk} = \delta_{ij}$ and $\sum_k u_{ik}v_{jk} + v_{ik}u_{jk} = 0$ to ensure that the transformation is canonical and preserves the anti-commutation relations. The inverse transformation is

$$\hat{\eta}_k = \sum_i u_{ik}\hat{c}_i + v_{ik}\hat{c}_i^\dagger \tag{105}$$

From the equations of motion for the operators $\hat{c}_i$ (or equivalently for $\hat{c}_i^\dagger$), the Bogoliubov transformation in Eq.104 and imposing the time dependence $\eta_k(t) = \eta_k e^{-i\Lambda_k t}$ for the normal modes, we obtain the following equations for the element of the transformation matrices u and v:

$$\begin{cases} \sum_j A_{ij}u_{jk} + B_{ij}v_{jk} = \Lambda_k u_{ik} \\ \sum_j B_{ij}u_{jk} + A_{ij}v_{jk} = -\Lambda_k v_{ik} \end{cases} \tag{106}$$

The Hamiltonian rewritten in terms of the normal modes reads $\hat{H} = \sum_k \Lambda_k \hat{\eta}_k^\dagger \hat{\eta}_k - \frac{1}{2}\sum_k \Lambda_k$.

We introduce the new matrices $\phi = u^T + v^T$ and $\psi = u^T - v^T$ whose column vectors satisfy the equations:

$$\begin{cases} (A+B)\,\vec{\phi}_k = \Lambda_k \vec{\psi}_k \\ (A-B)\,\vec{\psi}_k = \Lambda_k \vec{\phi}_k \end{cases} \tag{107}$$

They are real and such that $\phi^T\phi = 1$ and $\psi^T\psi = 1$. If $\Lambda_k \neq 0$, it is enough to solve the eigenvalue problem

$$M\vec{\psi}_k = \Lambda_k^2 \vec{\psi}_k \tag{108}$$

where the matrix $M = (A+B)(A-B)$ is positive, tridiagonal, and symmetric, and reads

$$M = \begin{pmatrix} b-\alpha & a & 0 & \cdots & 0 \\ a & b & a & \cdots & 0 \\ 0 & a & b & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & \cdots & a & b & a \\ 0 & \cdots & 0 & a & b-\beta \end{pmatrix}, \tag{109}$$

with $b = 4 + 4h^2$, $a = -4h$, $\alpha = 4h^2(1-\mu^2)$, $\beta = 4$, and so the spectrum of H_μ does not depend by the sign of μ.

By using the method in [106, 107], we see that the energies Λ_k can be written as

$$\Lambda_k = \Lambda(\theta_k) = \sqrt{b + 2a\cos(\theta_k)} = 2\sqrt{1 + h^2 - 2h\cos(\theta_k)} \tag{110}$$

where θ_k needs to satisfy the equation $f(\theta_k) = 0$ where $f(\theta)$ is the function

$$f(\theta) = a(\alpha+\beta)\sin(N\theta) + a^2 \sin\left[(N+1)\theta\right] + \alpha\beta\sin\left[(N-1)\theta\right] \tag{111}$$

Then the matrix ψ has elements

$$\psi_{kn} = \psi_n(\theta_k) = \mathcal{N}(\theta_k)\left(\alpha\sin[(n-1)\theta_k] + a\sin(n\theta_k)\right) \tag{112}$$

where $\mathcal{N}(\theta_k)$ is a normalization constant defined by $\sum_n(\psi_n(\theta_k))^2 = 1$ (the sign can be arbitrarily chosen).

The same results could be achieved from [108].

We note that the substitution $\theta_k \to -\theta_k$ returns the same eigenvalues Λ_k and the same matrix ψ.

If $\Lambda_k \neq 0$, then the matrix ϕ is obtained from

$$\vec{\phi}_k = \frac{1}{\Lambda_k}(A-B)\vec{\psi}_k \tag{113}$$

If $\Lambda_k = 0$, the correspondent vectors $\vec{\phi}_k$ and $\vec{\phi}_k$ can be calculated from

$$\begin{cases} (A+B)\,\vec{\phi}_k = 0 \\ (A-B)\,\vec{\psi}_k = 0 \end{cases} \tag{114}$$

and the relative phase between $\vec{\phi}_k$ and $\vec{\psi}_k$ can be chosen arbitrarily.

The determinant of $A+B$ (and also of $A-B$) is $(2h)^N\mu$, then for finite N, Eq. (114) admit solutions only if $\mu = 0$. The only solution is

$$\begin{cases} \psi_n^{(s)} = \sqrt{\frac{h^2-1}{1-h^{-2N}}}\, h^{-n} \\ \phi_n^{(s)} = \delta_{n,1} \end{cases} \tag{115}$$

so that ψ_n is localized near the first site if $h < 1$ or near the last site if $h > 1$. If $N \to \infty$ a solution exists if $h < 1$, also for $\mu \neq 0$, and it is calculated in the next subsection.

Since $\cos\theta_k$ needs to be real, we have to look only for the solutions of the non linear equation $f(\theta) = 0$ in θ, belonging to one of the three classes:

1. $\theta \in \mathbb{R}$
2. $\theta = 2m\pi + i\nu$, $\nu \in \mathbb{R}$, $m \in \mathbb{Z}$
3. $\theta = (2m+1)\pi + i\nu$, $\nu \in \mathbb{R}$, $m \in \mathbb{Z}$

5.A.1 Quasi-Continuum Spectrum

Let consider $\theta \in \mathbb{R}$.

If the real solution θ is such that $a(\alpha+\beta) + (a^2+\alpha\beta)\cos(\theta) \neq 0$, then from Eq. (111) it follows that θ is a solution of $\tan(N\theta) = \mathcal{F}(\theta)$, where the function $\mathcal{F}(\theta)$ is

$$\begin{aligned} \mathcal{F}(\theta) &= \frac{(\alpha\beta - a^2)\sin(\theta)}{a(\alpha+\beta) + (\alpha\beta + a^2)\cos(\theta)} \\ &= \frac{h\mu^2\sin(\theta)}{1-(\mu^2-1)h^2 + h(\mu^2-2)\cos(\theta)} \end{aligned} \tag{116}$$

The function $\mathcal{F}(\theta)$ is a periodic function of θ of period 2π, and it is also an odd function. Trivial solutions are $k\pi$, but they must be excluded because $\psi_n(k\pi) = 0$ from (112). Then it is enough to search the solutions θ_κ inside the interval $(0, \pi)$. They are such that

$$\theta_\kappa = \frac{1}{N}\left(\arctan(\mathcal{F}(\theta_\kappa)) + \kappa\pi\right) \tag{117}$$

The index κ is an integer number, and so θ_κ differs from $\frac{\kappa\pi}{N}$ by the $\mathcal{O}(N^{-1})$ function $\frac{1}{N}\arctan(\mathcal{F}(\theta_\kappa))$. Then, given a function $g(\theta)$

$$\frac{1}{N}\sum_\kappa g(\theta_\kappa) = \frac{1}{\pi}\int_0^\pi g(\theta)d\theta + \mathcal{O}(N^{-1})$$

if the limit of the Riemann sum exists and is finite.

All the solutions θ_κ can be labeled so that $\theta_\kappa \in I_\kappa = [\frac{(\kappa-1)\pi}{N}, \frac{\kappa\pi}{N}]$.

A solution θ_κ up to terms of the order $\mathcal{O}(N^{-2})$ can be obtained from Eq. (117), by evaluating the function $\mathcal{F}$ in Eq. (117) at a point θ_κ^0 in the interval I_κ.

$$\theta_\kappa = \frac{1}{N}\Big(\arctan(\mathcal{F}(\theta_\kappa^0)) + n_\kappa\pi\Big) + \mathcal{O}(1/N^2) \tag{118}$$

where n_κ is defined by the labeling chosen.

From Eq. (110) we have

$$\Lambda_\kappa = \Lambda(\theta_\kappa) = 2\sqrt{h^2 + 1 - 2h\cos(\theta)} \tag{119}$$

with $\theta_\kappa \in \mathcal{S} = \{\theta_\kappa : \kappa \in \mathcal{K}\}$ and

$$\mathcal{K} = \begin{cases} \{2, 3, \cdots, N\} & \text{if} \quad (h, \mu) \in (\mathcal{R}_1 \setminus \mathcal{R}_{2b}) \cup \mathcal{R}_{2a} \\ \{1, 2, \cdots, N-1\} & \text{if} \quad (h, \mu) \in \mathcal{R}_{2b} \\ \{1, 2, \cdots, N\} & \text{if} \quad (h, \mu) \notin \mathcal{R}_1 \cup \mathcal{R}_2 \\ \{2, 3, \cdots, N-1\} & \text{if} \quad (h, \mu) \in \mathcal{R}_1 \cap \mathcal{R}_2 \end{cases}$$

We have defined

$$
\begin{aligned}
\mathcal{R}_1 &= \{(h,\mu) : h \le 1\} & (120)\\
\mathcal{R}_{2a} &= \{(h,\mu) : h \ge 1 \wedge |\mu| \le \sqrt{1-h^{-1}}\} & (121)\\
\mathcal{R}_{2b} &= \{(h,\mu) : |\mu| \ge \sqrt{1+h^{-1}}\} & (122)\\
\mathcal{R}_2 &= \mathcal{R}_{2a} \cup \mathcal{R}_{2b} & (123)
\end{aligned}
$$

We can define the characteristic function χ_α of the domain $\mathcal{R}_\alpha$ as

$$
\chi_\alpha = \begin{cases} 1 & \text{if} \quad (h,\mu) \in \mathcal{R}_\alpha \\ 0 & \text{elsewhere} \end{cases}
$$

then n_κ can be written as

$$
n_\kappa = \kappa - \chi_1(1-\chi_{2b}) - \chi_{2a} - \Theta(\overline{\theta} - \theta^0_\kappa)\chi_1\chi_2 - \Theta(\theta^0_\kappa - \overline{\theta})(1-\chi_1)(1-\chi_2) \tag{124}
$$

where $\overline{\theta} = \arccos\left(\frac{(\mu^2-1)h^2-1}{(\mu^2-2)h}\right)$.

All the eigenvalues Λ_κ need to be inside the interval $I_b = [2\,|1-h|\,, 2\,|1+h|]$, and at the thermodynamic limit they densely cover I_b.

The corresponding matrix elements $\psi_{\kappa n}$ and $\phi_{\kappa n}$ are obtained from Eq. (112) and (113) respectively,

$$
\begin{cases}
\psi_{\kappa n} = \sqrt{\frac{2}{N}} \frac{\sin(n\theta_\kappa) + (\mu^2-1)h\sin((n-1)\theta_\kappa)}{\sqrt{1+(\mu^2-1)^2h^2+2h(\mu^2-1)\cos\theta_\kappa}} \\
\phi_{\kappa n} = \frac{2}{\Lambda_\kappa}\left(h\psi_{\kappa n} + \delta_{n,1}(\mu-1)h\psi_{\kappa n} - (1-\delta_{n,1})\psi_{\kappa n-1}\right)
\end{cases} \tag{125}
$$

and if $N \gg 1$ we can use θ_κ as given in Eq. (118).

These modes are manifestly spatially delocalized.

5.A.2 Discrete Spectrum

We consider the possibility to have complex solutions θ of $f(\theta) = 0$. These solutions lead to some eigenvalues $\Lambda(\theta) \notin I_b$.

Let consider $\theta = 2m\pi + i\nu$. We then have

$$\Lambda(\theta) = \sqrt{b + 2a\cosh(\nu)} = 2\sqrt{1 + h^2 - h\left(y + y^{-1}\right)} \tag{126}$$

where $y = e^{\nu}$. Since $\psi_n(\theta)$ given in (112), only gets a global phase under the transformation $\nu \to -\nu$, we consider $\nu \geq 0$.

We define $y_\infty = e^{\nu_\infty}$ where $\nu_\infty = \lim_{N\to\infty} \nu$. Then, in the limit $N \to \infty$ the equation $f(\theta) = 0$ becomes

$$y_\infty^2 + \frac{\alpha+\beta}{a} y_\infty + \frac{\alpha\beta}{a^2} = 0 \tag{127}$$

Only the solutions $y_\infty \geq 1$ are acceptable because $\nu > 0$.

We are considering $h > 0$, then there is only a solution acceptable if $(h, \mu) \in \mathcal{R}_1$ or if $(h, \mu) \in \mathcal{R}_{2a}$.

In the region $\mathcal{R}_1$ it reads $y_\infty = \frac{1}{h}$, and from Eq.(126) by using $\theta_\infty = 2m\pi + i\nu_\infty$, the eigenvalue $\Lambda_{(1)} = \Lambda(\theta_\infty)$ is zero at the thermodynamic limit, for every finite value of μ. Specifically

$$\Lambda_{(1)} \approx \frac{2\,|\mu|\,(1-h^2)}{\sqrt{1+(\mu^2-1)h^2}} h^N \tag{128}$$

because

$$y = e^{\nu_\infty} + \frac{\mu^2 h}{1+(\mu^2-1)h^2}\left(1 - e^{2\nu_\infty}\right) e^{-2N\nu_\infty}$$

at least to terms of the order $\mathcal{O}(e^{-4N\nu_\infty})$.

Then

$$\begin{cases} \psi_n^{(1)} = \psi_n(\theta) = \sqrt{1-h^2}\left(h^{N-n} - \frac{\mu^2}{1+(\mu^2-1)h^2} h^{N+n}\right) \\ \phi_n^{(1)} = \frac{\sqrt{1-h^2}}{|\mu|\sqrt{1+(\mu^2-1)h^2}} \left(1 + (\mu-1)\left(\delta_{n1} + (1-\delta_{n1})(1+\mu)\right)\right) h^{n-1} \end{cases} \tag{129}$$

Instead, in the region $\mathcal{R}_{2a}$ the solution to Eq. (127) reads $y_\infty = -h\left(\mu^2 - 1\right)$. From Eq. (126), in the thermodynamic limit the energy is

$$\Lambda_{(2)} = \Lambda(\theta_\infty) = 2\,|\mu|\sqrt{\frac{1+(\mu^2-1)h^2}{\mu^2-1}} \tag{130}$$

and from Eq. (112) and (113)

$$\begin{cases} \psi_n^{(2)} = \psi_n(\theta_\infty) = \sqrt{(\mu^2-1)^2h^2-1}(1-\mu^2)^{-n}h^{-n} \\ \phi_n^{(2)} = \frac{2}{\Lambda_{(2)}}\left(h\psi_n^{(2)} + \delta_{n,1}(\mu-1)h\psi_n^{(2)} - (1-\delta_{n,1})\psi_{n-1}^{(2)}\right) \end{cases} \tag{131}$$

If $\mu = 0$ the energy $\Lambda_{(2)}$ is zero, and $\phi_n^{(2)} = \delta_{n\,1}$, $\psi_n^{(2)} = h^{-n}\sqrt{h^2-1}$ where the relative sign between $\vec{\psi}^{(2)}$ and $\vec{\phi}_n^{(2)}$ can be chosen arbitrarily.

Let consider $\theta = (2m+1)\pi + i\nu$. We can proceed in a similar way to the previous case. We have

$$\Lambda(\theta) = 2\sqrt{1+h^2+h\left(y+y^{-1}\right)} \tag{132}$$

where $y = e^{\nu}$.

We put $\nu \geq 0$, then from $f(\theta) = 0$, in the limit $N \to \infty$ we have

$$y_\infty^2 - \frac{\alpha+\beta}{a}y_\infty + \frac{\alpha\beta}{a^2} = 0 \tag{133}$$

By the condition $y_\infty \geq 1$, there is only a solution acceptable if $(h,\mu) \in \mathcal{R}_{2a}$, and it reads $y_\infty = (\mu^2-1)h$.

The energy is $\Lambda_{(2)}$ given in Eq. (130), and the elements of matrices are given in Eq. (131).

5.B TRANSVERSE MAGNETIZATION

The transverse magnetization is defined by $\langle \hat{S}_n^z \rangle = \langle \frac{\sigma_n^z}{2} \rangle = \frac{1}{2} - \langle c_n^\dagger c_n \rangle$.

The average, respect the ground state, can be calculated with respect to the vacuum state $|\tilde{0}\rangle$

$$\langle c_n^\dagger c_n \rangle = \sum_k v_{nk}^2 = \frac{1}{4}\left(2\mathbb{1} - \phi^T\psi - \psi^T\phi\right)_{nn} = \frac{1}{2} - \frac{1}{2}\sum_k \phi_{kn}\psi_{kn}$$

and so

$$\langle \hat{S}_n^z \rangle = \frac{1}{2}\sum_k \phi_{kn}\psi_{kn}$$

We focus on the case $\mu \to 0$ and on the magnetization on the first site $\langle \hat{S}_1^z \rangle$. The contribution from the delocalized modes κ is $\phi_1(\theta)\psi_1(\theta) = \mathcal{O}(\mu)$, as can be seen from Eq. (125).

In the limit $N \to \infty$, if $h < 1$, the mode $\Lambda_{(1)}$ exists but its contribution goes to zero as h^N. Instead, if $h > 1$, the mode $\Lambda_{(2)}$ is important as it leads to a non zero contribution so that $\phi_1^{(2)}\psi_1^{(2)} \sim \frac{\sqrt{h^2-1}\mu}{h|\mu|}$ then

$$\lim_{\mu \to 0^\pm} \langle \hat{S}_1^z \rangle = \pm \frac{\sqrt{h^2-1}}{2h} \Theta(h-1) \tag{134}$$

Instead, for a finite N, at $\mu = 0$ the only non zero contribution comes from the mode with zero frequency in Eq. (115), and we have

$$\lim_{\mu \to 0^\pm} \langle \hat{S}_1^z \rangle = \pm \frac{1}{2h} \sqrt{\frac{h^2-1}{1-h^{-2N}}} \tag{135}$$

If the system is prepared in a thermal Gibbs state ρ_G at the temperature T, the transverse magnetization on the first site can be obtained from F by using

$$\langle \hat{\sigma}_1^z \rangle = -\frac{1}{h} \frac{\partial F(\mu)}{\partial \mu}$$

Where, in the thermodynamic limit,the derivative $\frac{\partial F(\mu)}{\partial \mu}$ is given in Eq. (94).

5.C QUANTUM ISING MODEL: TIME EVOLUTION AFTER A LOCAL QUENCH

Specifically, we consider the case for which the time evolution is generated by the Hamiltonian H_f, and the initial state $|\psi_i\rangle$ is a non equilibrium state prepared by performing the sudden quench $H_i \to H_f$, i.e. $|\psi_i\rangle$ is the ground state $|GS_i\rangle$ of the pre-quench Hamiltonian H_i.

We introduce the fermionic operators η_k and ξ_k by performing the Bogoliubov transformations

$$\hat{c}_i = \sum_k u_{ik}\hat{\eta}_k + v_{ik}\hat{\eta}_k^\dagger \quad (136)$$

$$\hat{c}_i = \sum_k w_{ik}\hat{\xi}_k + z_{ik}\hat{\xi}_k^\dagger \quad (137)$$

such that H_i and H_f expressed in terms of the operators $\{\eta_k, \eta_k^\dagger\}_k$ and $\{\xi_k, \xi_k^\dagger\}_k$ respectively are in their diagonal forms. We indicate with Λ_k the single particle energies of H_f. The new operators are related by the Bogoliubov transformation

$$\hat{\xi}_k = \sum_q U_{kq}\hat{\eta}_q + V_{kq}\hat{\eta}_q^\dagger$$

where

$$U_{kq} = \sum_i w_{ik}u_{iq} + z_{ik}v_{iq} \quad (138)$$

$$V_{kq} = \sum_i z_{ik}u_{iq} + w_{ik}v_{iq}$$

Then $\hat{c}_i(t) = e^{iH_f t}c_i e^{-iH_f t}$ is given by

$$\hat{c}_i(t) = \sum_k u_{ik}(t)\hat{\eta}_k + v_{ik}(t)\hat{\eta}_k^\dagger \quad (139)$$

where

$$u_{ik}(t) = \sum_q w_{iq}e^{-i\Lambda_q t}U_{qk} + z_{iq}e^{i\Lambda_q t}V_{qk} \quad (140)$$

$$v_{ik}(t) = \sum_q w_{iq}e^{-i\Lambda_q t}V_{qk} + z_{iq}e^{i\Lambda_q t}U_{qk} \quad (141)$$

We focus on the case $H_i = H_0$ and $H_f = H_1$, and we characterize the propagation of the perturbation by looking how the spatial profile of the transverse magnetization evolves in time. So we consider the difference $\delta m_i(t) = \langle \hat{S}_i^z \rangle_{GS_1} - \langle \hat{S}_i^z(t) \rangle_{GS_0} = \langle \hat{n}_i(t) \rangle_{GS_0} - \langle \hat{n}_i \rangle_{GS_1}$, where $\hat{n}_i = \hat{c}_i^\dagger \hat{c}_i$.

At the initial time $t = 0$, δm_i decays exponentially with the distance from the defect, $\delta m_i = \delta m_1 \exp(-(i-1)/\xi)$, with a short localization length ξ, see Fig. 5.C.1.

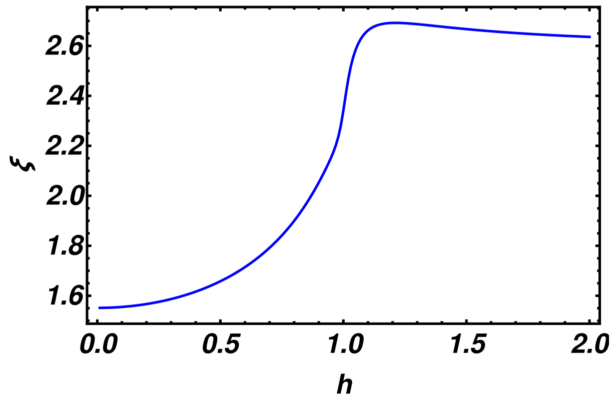

Figure 5.C.1.: The graphic shows the behavior of the localization length ξ. We put $N = 100$.

Notice, in particular, that the perturbation is always localized within the first three sites regardless of the value of h. On the other hand, δm_1 increases with h for $0 < h < 1$ while it goes to zero for $h > 1$ away from the critical point (indeed, in the paramagnetic phase, the magnetization tends to saturate with increasing h, both with and without the defect).

At the time t, the mean local number of fermions at site i is

$$\langle \hat{n}_i(t) \rangle_{GS_0} = \langle \hat{n}_i \rangle_{GS_1} + \sum_{k_1,k_2} A^{(i)}_{k_1 k_2} \cos\left(\left(\Lambda_{k_1} - \Lambda_{k_2} \right) t \right) \tag{142}$$

$$+ \sum_{k_1,k_2} B^{(i)}_{k_1 k_2} \cos\left(\left(\Lambda_{k_1} + \Lambda_{k_2} \right) t \right) \tag{143}$$

where

$$A^{(i)}_{k_1 k_2} = \left(w_{ik_1} w_{ik_2} - z_{ik_1} z_{ik_2} \right) \sum_l V_{k_1 l} V_{k_2 l} \tag{144}$$

$$B^{(i)}_{k_1 k_2} = 2 z_{ik_1} w_{ik_2} \sum_l U_{k_1 l} V_{k_2 l}. \tag{145}$$

In order to characterize the propagation of the perturbation in the magnetization profile, we consider the mean square magnetization center and its velocity defined as

$$R^2(t) = \sum_i \delta m_i(t)(i-1)^2 \tag{146}$$

$$v(t) = \frac{d}{dt}\sqrt{|R^2(t) - R^2(0)|} \tag{147}$$

We have that

$$R^2(t) = \sum_{k_1 k_2} A_{k_1 k_2} \cos\left((\Lambda_{k_1} - \Lambda_{k_2})t\right) + B_{k_1 k_2} \cos\left((\Lambda_{k_1} + \Lambda_{k_2})t\right) \tag{148}$$

where

$$A_{k_1 k_2} = \sum_i A^{(i)}_{k_1 k_2}(i-1)^2 \tag{149}$$

$$B_{k_1 k_2} = \sum_i B^{(i)}_{k_1 k_2}(i-1)^2 \tag{150}$$

The Lieb-Robinson bound can be studied by considering the imaginary part of the time-dependent correlation function $\rho^{zz}_{ij}(t) = \langle \sigma^z_i(t)\sigma^z_j(0)\rangle$

$$\mathrm{Im}\rho^{zz}_{ij}(t) = 4\mathrm{Im}\langle n_i(t) n_j(0)\rangle \tag{151}$$

With respect to the initial state chosen, we have

$$\mathrm{Im}\langle n_i(t) n_j(0)\rangle = \sum_{k_1 k_2} C^{ij}_{k_1 k_2} \sin\left(\left(\Lambda_{k_1} - \Lambda_{k_2}\right)t\right) + D^{ij}_{k_1 k_2} \sin\left(\left(\Lambda_{k_1} + \Lambda_{k_2}\right)t\right) \tag{152}$$

6 THE DRIVEN DICKE MODEL

The dynamical behavior of quantum critical systems displays interesting features concerning defects or excitations production, which occurs when the system is driven across its critical point.

In this Chapter we outline the study of another critical system, the so-called Dicke model [109], representing a paradigmatic example in ethis context. The model describes a system of free atoms that interact with a bosonic mode. It shows a thermodynamic phase transition if the coupling is large enough. The system is brought out of the equilibrium by a parametric driving [D]. We study the dynamics in general, with a particular emphasis on the work performed because of the driving. The non adiabaticity property, induced by the driving, is characterized in terms of the inner friction, that has been previously studied in the Sec. 3.2.

The Dicke model is introduced in Sec. 6.1, where the phase transition is briefly discussed.

In Sec. 6.2 the dynamics is studied in general, by using a perturbative approach that tends to be exact at the thermodynamic limit, in which the dynamics is described by a Gaussian propagator. The study is done in terms of classical mean-fields, and quantum fluctuations operators. It is shown how an instable behavior can arise, as discussed in detail in Sec. 6.2.1, in which the quantum fluctuations undergo an unbounded amplification. This behavior, as studied for a linear driving, could lead to an exponential generation of the quantum correlations between the two subsystems, quantified by the logarithmic negativity. The exponential growth is abruptly interrupted as the non linear terms become active, leading to a coarse grained saturation in the quantum correlations.

We carry on our analysis, by focusing on a periodic driving in Sec. 6.3. For this particular case, the dynamics is characterized with the help of a stability diagram, obtained by using the Floquet theorem. Photons could be generated by a parametric amplification of the vacuum fluctuations, and in Sec. 6.3.1 this mechanism is linked to the work done on the system. Furthermore, during the driving, the system is typically unable to follow its instantaneous equilibrium state. This effect is described by considering the inner friction produced in the process.

In Sec. 6.3.2, it is shown how the quantum fluctuations can be characterized by using some figures of merit. In particular, we focus on the Mandel parameter and the degree of two-mode squeezing.

6.1 THE DICKE MODEL

The Dicke Model (DM) describes a system of a N two-level atoms interacting collectively with a single bosonic mode. Originally, the DM was introduced to describe the coupling of N two-level atoms with an electromagnetic field [109]. The model is defined by the Hamiltonian $\hat{H} = \hat{H}_0 + \hat{H}_{int}$ with

$$\hat{H}_0 = \omega_a \hat{a}^\dagger \hat{a} + \omega_b \hat{J}_z \,, \quad \hat{H}_{int} = 2g\left(\hat{a}^\dagger + \hat{a}\right)\hat{J}_x/\sqrt{N}. \tag{153}$$

Here $\hat{a}$ ($\hat{a}^\dagger$) is a bosonic annihilation (creation) operator, and $\hat{\boldsymbol{J}} = (\hat{J}_x, \hat{J}_y, \hat{J}_z)$ is the collective spin operator, with $\hat{\boldsymbol{J}} = \sum_{i=1}^{N} \hat{\boldsymbol{\sigma}}_i/2$ and $\hat{\boldsymbol{\sigma}}_i$ is the vector of Pauli spin operators.

Since the total spin $\hat{\boldsymbol{J}}^2$ is conserved, the states $\{|j,m\rangle\}$ [110] defined as

$$\begin{aligned}\hat{\boldsymbol{J}}^2 |j,m\rangle &= j(j+1)\,|j,m\rangle \\ \hat{J}_z\,|j,m\rangle &= m\,|j,m\rangle\end{aligned}$$

play a key role in the Dicke theory, and they take the name of super radiant states [109]. Explicitly, the subspaces of the Hilbert space of the system, with a given j are dynamically invariant. The quantum number j is the so-called cooperation number [109], and it has been shown how coherent radiation can be emitted when j is large while m is small.

Another important constant of motion is the parity, which, in the subspace with a given j, reads $\hat{\Pi} = \exp\{i\pi(\hat{a}^\dagger \hat{a} + \hat{J}_z + j)\}$, where $\hat{a}^\dagger \hat{a} + \hat{J}_z + j$ gives the number of excitations in the state of the whole system [111].

By taking advantage of the parity symmetry, the model with $N = 1$, taking the name of Rabi model [112], was recently solved [113, 114] in the Bargmann representation [115].

Here, we focus on the large N limit. In the thermodynamic limit, if the atom-photon coupling g is larger than the critical value

$$g_c = \sqrt{\omega_a \omega_b}/2\,, \tag{154}$$

then there exists a critical temperature $T_c = (k_B \beta_c)^{-1}$, given by [116]

$$\tanh\left(\frac{\beta_c}{2}\right) = \frac{\omega_a \omega_b}{4g^2} = \mu\,, \tag{155}$$

at which the DM undergoes a thermodynamic phase transition, generally referred to as the Super-Radiant (SR) transition.

When the temperature decreases crossing T_c, the system goes from its Normal (N) phase to the SR phase, that is a macroscopically excited and highly collective state that possesses the potential to super-radiate [117].

This phase transition was firstly studied by Hepp and Lieb [118] under the Rotating-Wave Approximation (RWA), with the interaction described by $\hat{H}_{int}^{(RWA)} = g\left(\hat{a}^\dagger \hat{J}_- + \hat{a}\hat{J}_+\right)/\sqrt{N}$. Later, another procedure was provided by Wang and Hioe [119], that is formally justified in [120], where it is also shown that the super-radiant transition survives without the RWA.

The SR transition can be inhibited if quadratic terms in $\hat{a}$ and $\hat{a}^\dagger$ are taken into account in the Hamiltonian in Eq. (153) as shown in [121]. Specifically, in the original physical system [109, 118], the SR transition is always prohibited [121], because of the Thomas-Reiche-Kuhn sum rule [122, 123, 124, 125].

This no-go theorem can be bypassed by an engineering of the Hamiltonian H of the DM. For instance, the phase transition has been observed in a open

DM simulated thanks to a Bose-Einstein condensate coupled to an optical cavity [126], or by using ultracold atoms [127].

Recently, the QPT at $T_c = 0$ and the quantum-chaotic properties of the DM, have been studied in [111] by using a Holstein-Primakoff (HP) representation [128] for the atomic system.

Below the coupling g_c given in Eq. (154), i.e. if $\mu > 1$, where μ is defined in Eq. (155), the behavior imposed by the free Hamiltonian $\hat{H}_0$ is prevalent, and essentially there are no excitations in the ground state (N phase). Conversely, above g_c, the interaction is predominant, and the two subsystems get macroscopically populated. Their state then is well described by a displaced coherent state (SR phase) [111], but two equivalent values for the mean field could be choosen, giving rise to the phenomenon of the spontaneous symmetry breaking.

Despite being a ground state property, the existence of a phase transition point can play a crucial rule also in the time evolution of the system. In general, a dynamical phase transition [129] can occur by driving the system from a static phase to the other, as it was experimentally observed in the open DM [130].

For the particular case of a monochromatic non-adiabatic modulation of the atom-field coupling, it is shown that the DM shows a set of nonequilibrium quantum phase transitions [131].

6.2 DYNAMICS OF THE DRIVEN DICKE MODEL

We study the dynamics of the system allowing a time dependence in all the parameters $\omega_{a,b}$, and g (in order to avoid notational clutter, and unless otherwise specified, we will avoid writing explicitly any time dependence).

In order to give a simple theoretical description of the DM, we consider only the totally symmetric subspace, determined by $j = N/2$. For instance, this choice is justified if the atoms can be treated as indistinguishable, or if the initial state of the system belongs to this subspace.

Each spin operator restricted to the symmetric subspace $j = N/2$ is mapped into a bosonic mode thanks to the HP transformation

$$\hat{J}_z = \hat{b}^\dagger \hat{b} - N/2\,, \quad \hat{J}_+ \equiv \hat{J}_x + i\hat{J}_y = \hat{b}^\dagger \sqrt{N - \hat{b}^\dagger \hat{b}}. \tag{156}$$

where $\hat{b}$ and $\hat{b}^\dagger$ are bosonic operator such that $[\hat{b}, \hat{b}^\dagger] = 1$.

In this representation, as $N \to \infty$, the state $\left|\frac{N}{2}, n - \frac{N}{2}\right\rangle$ corresponds to the bosonic number state $|n\rangle$, and so the state $\mathcal{N}\sum_{n=0}^{N} \frac{\alpha^n}{\sqrt{n!}} \left|\frac{N}{2}, n - \frac{N}{2}\right\rangle$ corresponds to the coherent bosonic state $|\alpha\rangle$ [132].

The Hamiltonian that rules the free evolution of the two subsystems reads $\hat{H}_0 = \omega_a \hat{a}^\dagger \hat{a} + \omega_b \left(\hat{b}^\dagger \hat{b} - \frac{N}{2}\right)$, and the interaction $\hat{H}_{int}$ takes the form

$$\hat{H}_{int} = g\left(\hat{a}^\dagger + \hat{a}\right)\left(\hat{b}^\dagger \sqrt{1 - \frac{\hat{b}^\dagger \hat{b}}{N}} + \sqrt{1 - \frac{\hat{b}^\dagger \hat{b}}{N}}\,\hat{b}\right). \tag{157}$$

The atomic medium is described by an effective bosonic mode b non linearly interacting with the cavity mode, so that solving the dynamics in general is non trivial.

In the thermodynamic limit, the ground state of $\hat{H}$ and the low energy excitations can be calculated by isolating from $\hat{b}$ and $\hat{b}^\dagger$ macroscopic ($\sim \sqrt{N}$) mean contributions [111] and retaining only the leading terms of a $1/\sqrt{N}$ expansion of the non linear term in the interaction in Eq. (157). This procedure implies subtracting a *static* mean field chosen in order to approximate the Hamiltonian as accurately as possible at low energies.

Then, if the model is undriven, the time evolution of low energy states can be determined by finding the energy eigenstates involved.

Instead, for a driven model, this approach is less helpful as the evolution becomes non adiabatic.

Here, we describe the dynamics in general, by requiring that any macroscopic contribution is ascribed to time-dependent mean fields.

Under this ansatz, the bosonic operators a and b at a time t reads

$$\begin{cases} \hat{a}(t) = \sqrt{N}\alpha(t) + \hat{c}(t) \\ \hat{b}(t) = \sqrt{N}\beta(t) + \hat{d}(t)\,, \end{cases} \tag{158}$$

where the rescaled mean fields α and β are defined by

$$\begin{cases} \alpha(t) = \lim_{N\to\infty}\langle\hat{a}(t)\rangle/\sqrt{N} \\ \beta(t) = \lim_{N\to\infty}\langle\hat{b}(t)\rangle/\sqrt{N} \end{cases} \tag{159}$$

and remain $\mathcal{O}(1)$ as $N \to \infty$ (as it is the case for a static $\hat{H}$ [111]). Then bosonic operators $\hat{c}$ and $\hat{d}$, describing deviations from the macroscopic mean fields, satisfy the relations $[\hat{c}, \hat{c}^\dagger] = 1$, $[\hat{d}, \hat{d}^\dagger] = 1$, and their averages remain $\mathcal{O}(1)$ as well as $N \to \infty$.

With this ansatz, a perturbative study in the parameter $1/\sqrt{N}$ can be performed, and by using the leading terms only, the generator of the time evolution is described by the quadratic time-dependent Hamiltonian [1]

$$\begin{aligned} H_{\alpha,\beta} \;=\; & \omega_a c^\dagger c + \left[\omega_b - 2g\frac{\alpha_r\beta_r}{\sqrt{\Gamma}}\left(2 + \frac{|\beta|^2}{2\Gamma}\right)\right] d^\dagger d + g\sqrt{\Gamma}(c^\dagger + c) \times \\ & \left[\left(1 - \frac{\beta^*\beta_r}{\Gamma}\right) d + h.c.\right] - g\frac{\alpha_r}{\sqrt{\Gamma}}\left[\beta^*\left(1 + \frac{\beta^*\beta_r}{2\Gamma}\right) d^2 + h.c.\right] + \\ & \sqrt{N}\Bigg\{ \left(\omega_a\alpha + 2g\sqrt{\Gamma}\beta_r\right) c^\dagger + \left[\omega_b\beta + 2g\sqrt{\Gamma}\alpha_r\left(1 - \frac{\beta\beta_r}{\Gamma}\right)\right] d^\dagger + \\ & h.c.\Bigg\} + \Lambda_N \end{aligned} \tag{160}$$

up to terms of the order of $1/\sqrt{N}$, where $\Gamma = 1 - |\beta|^2$ is assumed to stay positive during the time evolution [111], while Λ_N is the c-number

$$\Lambda_N = N\left\{\omega_a|\alpha|^2 + \omega_b\left(|\beta|^2 - \frac{1}{2}\right) + 4g\sqrt{\Gamma}\alpha_r\beta_r\right\} - g\alpha_r\beta_r\frac{|\beta|^2}{2\sqrt{\Gamma}} \tag{161}$$

The rescaled mean fields α and β in Eq. (160) are obtained as solutions of the equations [2]

$$\begin{cases} i\dot{\alpha} = \omega_a\alpha + 2g\sqrt{\Gamma}\beta_r \\ i\dot{\beta} = \omega_b\beta + 2g\sqrt{\Gamma}\alpha_r\left(1 - \beta\beta_r/\Gamma\right) \end{cases} \tag{162}$$

1 Here $s_r = \mathrm{Re}(s)$ and $s_i = \mathrm{Im}(s)$ with $s = \alpha, \beta$.

2 In order to derive the values for α and β, we require that the time evolution generated by $H_{\alpha,\beta}$ leaves the operators c and d of order $\mathcal{O}(1)$ as $N \to \infty$, at any finite time t.

with initial conditions determined by the initial mean values of a and b. For instance, for the initial state with no photons in cavity and all the atoms excited, we have $\alpha(0) = 0$ and $\beta(0) = 1$.

If we regard α_r and β_r as the generalized coordinates, and α_i and β_i as their conjugate momenta, Eq. (162) can be derived from the effective Hamiltonian function

$$H(\alpha, \beta) = \frac{\omega_a}{2}|\alpha|^2 + \frac{\omega_b}{2}|\beta|^2 + 2g\sqrt{\Gamma}\beta_r\alpha_r$$

In the strict thermodynamic limit, thus, the Hamiltonian becomes quadratic, so that the time evolution can be described by a Gaussian propagator.

The Heisenberg equations for c and d are best displayed in terms of the quadrature vector $\hat{\boldsymbol{Q}} = (\hat{q}_c, \hat{q}_d, \hat{p}_c, \hat{p}_d)$ with $\hat{q}_k = (\hat{k} + \hat{k}^\dagger)/\sqrt{2}$, $\hat{p}_k = i(\hat{k}^\dagger - \hat{k})/\sqrt{2}$ $(k = c, d)$. In the limit $N \to \infty$, we have

$$\dot{\hat{\boldsymbol{Q}}} = \boldsymbol{M}_{\alpha,\beta}\,\hat{\boldsymbol{Q}}\,, \tag{163}$$

where matrix $\boldsymbol{M}_{\alpha,\beta}$ is a non-linear function of the instantaneous mean field values α and β, and it is given by

$$M_{\alpha,\beta} = \begin{pmatrix} 0 & 0 & \omega_a & 0 \\ -\frac{2g\beta_r\beta_i}{\sqrt{\Gamma}} & -\frac{2g\alpha_r\beta_i}{\sqrt{\Gamma}}\left(1 + \frac{\beta_r^2}{\Gamma}\right) & 0 & \omega_b - \frac{2g\alpha_r\beta_r}{\sqrt{\Gamma}}\left(1 + \frac{\beta_i^2}{\Gamma}\right) \\ -\omega_a & -2g\sqrt{\Gamma}\left(1 - \frac{\beta_r^2}{\Gamma}\right) & 0 & 2g\frac{\beta_r\beta_i}{\sqrt{\Gamma}} \\ -2g\sqrt{\Gamma}\left(1 - \frac{\beta_r^2}{\Gamma}\right) & -\omega_b + \frac{2g\alpha_r\beta_r}{\sqrt{\Gamma}}\left(3 + \frac{\beta_r^2}{\Gamma}\right) & 0 & \frac{2g\alpha_r\beta_i}{\sqrt{\Gamma}}\left(1 + \frac{\beta_r^2}{\Gamma}\right) \end{pmatrix} \tag{164}$$

In general, Eq. (163) are formally solved as $\hat{\boldsymbol{Q}}(t) = \Phi(t)\hat{\boldsymbol{Q}}(0)$, where matrix Φ is the solution of the differential equation $\dot{\Phi} = \boldsymbol{M}_{\alpha,\beta}\Phi$ with the initial condition $\Phi(0) = \mathbb{1}$.

Then the dynamics of the quantum fluctuations around the mean values $\langle a\rangle$ and $\langle b\rangle$ depends on the time evolution of mean fields α and β.

The Eq. (162) are manifestly nonlinear. However, by starting from low-energy conditions with respect to the free Hamiltonian H_0, the dynamics can be well approximated by linear equations of motion up until the time t_{lin}, within which $|\alpha|, |\beta| \ll 1$. In such *linear transient*, we have

$$\frac{d}{dt}\begin{pmatrix}\alpha_r\\ \beta_r\\ \alpha_i\\ \beta_i\end{pmatrix} \simeq M_0 \begin{pmatrix}\alpha_r\\ \beta_r\\ \alpha_i\\ \beta_i\end{pmatrix}, \qquad M_0 = \begin{pmatrix} 0 & 0 & \omega_a & 0\\ 0 & 0 & 0 & \omega_b\\ -\omega_a & -2g & 0 & 0\\ -2g & -\omega_b & 0 & 0\end{pmatrix} \tag{165}$$

and $\dot{\boldsymbol{Q}} \simeq M_0 \boldsymbol{Q}$, so that the quantum fluctuations and the mean fields have the same dynamics, as it is evident from Eq. (165).

When the mean fields acquire macroscopic values, their dynamics becomes fully non linear and the whole of Eq. (162) should be retained. For a constant Hamiltonian and any value of μ, Eq. (162) have the stationary solution $\alpha^{(n)} = \beta^{(n)} = 0$, corresponding to the mean fields of the N phase [111]. In the SR-phase, with $\mu < 1$, two other stationary points appear, corresponding to states with broken (parity) symmetry [111],

$$\begin{cases} \alpha_{\pm}^{(sr)} = \pm\frac{g}{\omega_a}\sqrt{1-\mu^2} \\ \beta_{\pm}^{(sr)} = \mp\sqrt{\frac{1-\mu}{2}} \end{cases} \tag{166}$$

For a driven system, μ depends on time and so do $\alpha^{(sr)}$ and $\beta^{(sr)}$ in Eq. (166), while the normal point $(\alpha^{(n)}, \beta^{(n)})$ is instead stationary. As a result, if the initial state has null mean values $\langle a(0)\rangle = \langle b(0)\rangle = 0$, the condition $\alpha = \beta = 0$ will hold at all times and the dynamics will never exit the linear transient.

However, if the system is instantaneously brought into the SR region, such normal stationary point becomes unstable.

Then, when the system is initially prepared in its N phase, small perturbations in the mean fields stay bounded and of the same order in time; but, if the system is instantaneously brought into the SR region, even a small perturbation gets an exponential amplification.

This behavior can be linked to the Kibble-Zurek mechanism [6, 7], that depicts the scenario of defects generation, when the system is drived towards a final phase characterized by a spontaneous symmetry breaking.

As discussed in [7], during the crossing of the phase transition point the state of the system tends to be “freezed”, because the relaxation times tend to diverge at this point (impulsive regime). We expect that the time t_{lin} could play the role of freeze-out time of the Kibble-Zurek theory [7].

As an example of such a behavior, we consider a linear driving.

The system is driven towards the SR region, by changing the coupling as $g(t) = g_c\left(1 + \frac{t}{\tau}\right)$, in the time interval $[-\tau, \tau]$.

Initially the radiation field has been taken in the coherent state $|\sqrt{N}\epsilon\rangle$ with $\epsilon \ll 1$, and all of the atoms in their ground states.

For this case, we have characterized the entanglement generation between the atomic system and the electromagnetic mode, described by the logarithmic negativity E_N [133, 134].

As the system enters in the SR region, there is an exponential growth of the entanglement, until a time t^* when it starts to decrease, and the non linear terms become active. As ϵ goes to zero, t^* goes to infinity.

After this time, the logarithmic negativity E_N fluctuates, yet remaining of the same order. This behaviour is illustred in Fig. 6.2.1 (left panel). The time t^* shows non analytic points as a function of the driving time τ, at regular intervals as shown in Fig. 6.2.1 (right panel).

6.2.1 Limits of Validity and Instability Rate γ^*

Our description of the dynamics becomes exact for every finite time t in the limit $N \to \infty$. Anyway, it’s crucial to understand what the limits of applicability of our approach are for finite N.

For finite N, one should consider further terms in the expansion in Eq. (160), in order to achieve a more accurate description.

We have seen that during the time evolution, the fluctuations can become very large and even unbounded in time.

For finite but large N our description stays accurate until the n^{th} moment of $\boldsymbol{Q}$ becomes of order $N^{n/2}$.

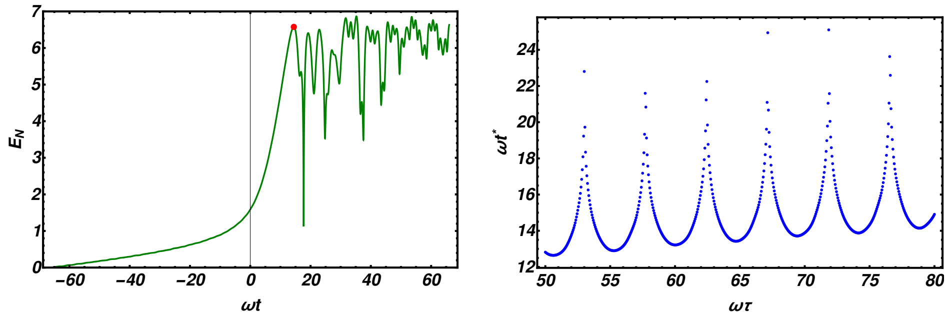

Figure 6.2.1.: (Color online): Left: Logarithmic negativity E_N as a function of time. As the system is driven towards the SR region, by changing the coupling as $g(t) = g_c\,(1 + \frac{t}{\tau})$, in the time interval $[-\tau, \tau]$. We consider an initial state $\left|\sqrt{N}\epsilon\right\rangle |N/2, -N/2\rangle$, with $\epsilon = 10^{-2}$. There is an exponential growth, that ends near the time t^*, when the entanglement reaches the first maximum (red point), and then it stays of the same order. Here we have chosen $\omega_a = \omega_b = \omega$ and $\tau = 66\omega$.
Right: The time t^* as a function of τ.

To ensure that this is not the case, it is enough to require that all of the elements of the matrix Φ are small compared to $\sqrt{N}$. Therefore, our description of the dynamics is accurate until a time t_{max}, defined as the first instant for which

$$max_{ij}\,\{\Phi_{ij}(t_{max})\} \approx \sqrt{N} \tag{167}$$

In the limit $N \to \infty$, we expect $t_{max} \to \infty$, since the dynamics of $\boldsymbol{Q}$ is independent of N (see Eq. (164)).

In order to characterize and estimate t_{max}, we need to consider the initial conditions for the mean fields, $\alpha(0) = \alpha_0$ and $\beta(0) = \beta_0$. In particular, if we take $\delta = max\,\{|\alpha_0|, |\beta_0|\} \ll 1$, the first part of the dynamics is included in the linear transient. This implies that, for $0 \leq t < t_{lin}$, the time evolution of both the fluctuations and the mean-fields is determined by the linearized matrix M_0.

In the absence of driving and in the linear transient, the dynamics would be characterized by the eigenvalues of the matrix M_0. Two of them are always purely imaginary, i.e. $\pm i\lambda_1$. The other two are $\pm i\lambda_2$, where λ_2 is real if $\mu > 1$, it is equal to λ_1 if $\mu = 1$ and it is purely imaginary if $\mu < 1$. This means that if $\mu > 1$ the fluctuations and the mean fields stay always of the same order, i.e $t_{lin} \to \infty$ and $t_{max} \to \infty$. At the transition point, $\mu = 1$, fluctuations and mean-fields grow linearly in time; while in the super-radiant phase $\mu < 1$, the fluctuations and the mean fields can experience an exponential growth, with an *instability rate* given by $\gamma^* = |\lambda_2|$. This is true until $t \lesssim t_{lin}$. After t_{lin}, the nonlinear terms cannot be neglected anymore and one has to consider the full non-linear equations. Thus, within the linear regime, we can define the characteristic time τ^* as the inverse of the instability rate, i.e.

$$\tau^{*-1} = \gamma^* = \sqrt{\sqrt{\left(\frac{\omega_a^2 - \omega_b^2}{2}\right)^2 + 4\omega_a\omega_b g^2} - \frac{\omega_a^2 + \omega_b^2}{2}}$$

If $\delta = 0$, then $t_{lin} \to \infty$ and the time of validity t_{max} is given by the condition $e^{\gamma^* t_{max}} \approx \sqrt{N}$, and so $t_{max} \approx \frac{\tau^*}{2} \ln(N)$.

If $\delta \neq 0$, we can estimate t_{lin} as the time for which one of the mean fields (either α or β) becomes of the order of one,

$$t_{lin} \approx \tau^* \ln\left(\delta^{-1}\right) \tag{168}$$

Since $\delta \ll 1$, we expect t_{lin} to be much larger than τ^*.

The crucial point, however, is wether or not all of the linear transient is contained within our limit of validity. Indeed, for this description to be valid for times of the order of t_{lin}, we have to require that $e^{\gamma^* t_{lin}} \ll \sqrt{N}$, from which it follows that $t_{lin} \ll \frac{\tau^*}{2} \ln(N)$, and by using Eq. (168), $\delta \gg \frac{1}{\sqrt{N}}$.

This condition is always fulfilled, because the contributions at the averages $\langle a \rangle$ and $\langle b \rangle$ of the order $\frac{1}{\sqrt{N}}$ are taken in account with $\langle c \rangle$ and $\langle d \rangle$. Then $t_{lin} \ll t_{max}$, and our description makes full sense even outside the linear transient, and can be used even when the mean fields take values of the order of $\sqrt{N}$. Anyway, it is not possible to give a simple expression for t_{max}, as it depends on the non-linear terms appearing in the time evolution, and the only way to check the validity of our approach is to check the condition (167).

These estimates and reasoning can be adapted also to the case of a driven system, since they are simply a consequence of the fact that the dynamics of the mean fields and that of the fluctuations are the same in the linear transient.

For instance, for a periodically driven Hamiltonian, we can use the largest positive Floquet exponent of the linearized matrix M_0 in order to estimate τ^*; and then use again the equations above to estimate t_{lin} and t_{max}. Specifically, if M_0 is periodic in time, with period T, then the monodromy matrix (in the Floquet description [135]) is given by $\mathcal{M} = \Phi(T)$. The eigenvalues of $\mathcal{M}$ are the Floquet multipliers $\{\rho_i\}_{i=1}^4$. From these, we can calculate the Floquet exponents, that are the complex numbers $\nu_i = \frac{\ln(\rho_i)}{T}$. So we can define the instability rate γ^* as the maximum among zero and the real parts of the Floquet exponents, i.e.

$$\gamma^* = max\left\{0,\ \{\mathbb{R}e\{\nu_i\}\}_{i=1}^4\right\} \tag{169}$$

As a result, the arguments above can be applied in this case too, even if, in a strict sense, the stability of the dynamics cannot be fully characterized by the instantaneous eigenvalues of the matrix M_0.

6.3 PERIODIC DRIVING

In the following, we focus on a periodically driven system, leading to a parametric amplification of the vacuum fluctuations [136], mimicking the dynamical Casimir effect [137, 138]. Specifically, the atomic frequency is assumed to be sinusoidally perturbed, $\omega_b/\omega_a = \lambda_0 + \lambda \sin(\eta t)$, implying an harmonic time dependence for $\mu(t)$, which oscillates between $\mu_{min} = \mu_0(1 - \lambda/\lambda_0)$ and $\mu_{max} = \mu_0(1 + \lambda/\lambda_0)$, with amplitude $\mu_0 = \lambda_0\omega_a^2/4g^2$ and frequency η.

For such a periodic driving, we make use of Floquet theory [135, 47] to study the dynamics of the system in the linear transient. In particular, the stability of the solutions of Eq. (162) can be characterized by an instability rate γ^* defined as the largest positive Floquet exponent of the linearized equations [135], which embodies the growing rate of the mean fields in the linear regime. While the details of this analysis are given in the previous section and the result is reported in Fig. 6.3.1, where we see that $\gamma^* > 0$ if $\mu(t) < 1$ at all times (above the black line in Fig. 6.3.1), while driving-induced instabilities appear even when $\mu(t) > 1$ at all times (below the green line in Fig. 6.3.1). For small couplings, this occurs near the parametric resonance points $\eta_k = \omega_a(1 + \lambda_0)/k$

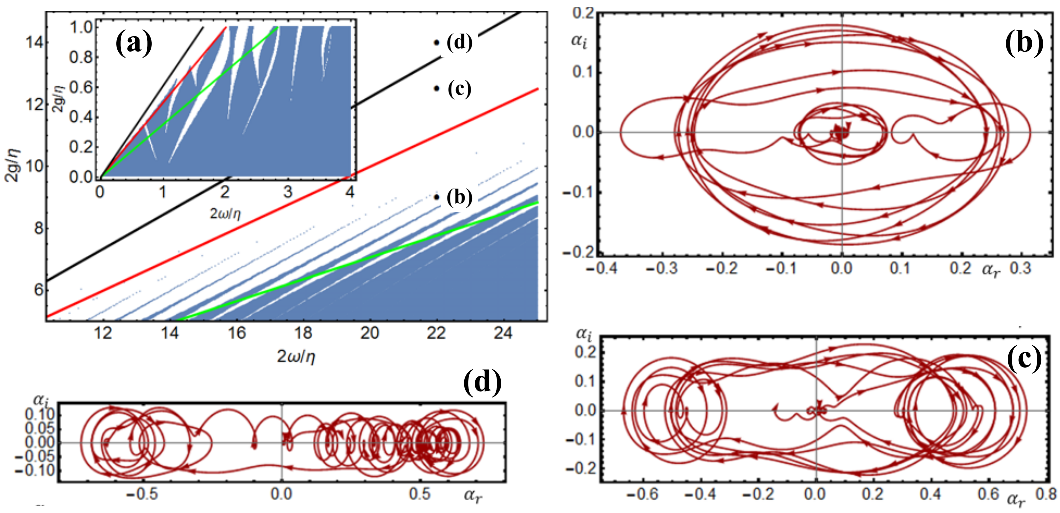

Figure 6.3.1.: (Color online) **(a)** Stability diagram in the driving frequency vs. coupling plane, signalling in white the regions with positive instability rate, $\gamma^* > 0$. The plot is drawn at the static resonance, $\omega_a = \omega_b(0) = \omega$, with $\lambda = \frac{1}{2}$. The red line signals the static critical coupling $\mu_0 = 1$, and for a sufficiently fast driving, $\gamma^* < 0$ below this line. Instead, the black line corresponds to $\mu_{max} = 1$, so that, for a point over the black line $\mu(t) < 1 \forall t$ and $\gamma^* > 0$. Finally, the green one is $\mu_{min} = 1$, so that, for a point under the green line $\mu(t) > 1 \forall t$, inside of which the white zones open for $\eta_k = 2\omega/k$, $k \in Z$, as $g \to 0$. The inset shows the stability diagram for larger values of the driving frequency. **(b)-(d)** Trajectories of the mean field α corresponding to the three points in panel **(a)**. We have assumed a slow periodic driving ($\omega_a = 11\eta$) and evaluated $\alpha(t)$ up to $t = 60\eta^{-1}$ by numerically solving Eqs. (162) for the parameters indicated by the black dots in the central panel, with $2g/\eta = 9, 12.5, 14$. Initially, the radiation field has been taken in the coherent state $|\sqrt{N}\epsilon\rangle$ with $\epsilon = 10^{-2}$, with all of the atoms in their ground states.

($k \in \mathbb{Z}$). These are the so called Arnold instability tongues, discussed in [131], and studied there as $g \to 0$ by using a perturbative approach.

Although the dynamics can exit the linear regime when the mean fields acquire large values (which can occur quite quickly, e.g., for initial coherent states with very small amplitudes), the diagram in Fig. 6.3.1 still helps classifying the dynamical behavior of the mean fields, identifying those values of frequency and coupling for which α and β grow exponentially in time, from those for which they stay bounded.

Clearly, the same diagram will help also in the study of quantum fluctuations. In particular, for a parameter set in the white region, the dynamics of the fluctuations becomes chaotic, since the matrix $\boldsymbol{M}_{\alpha,\beta}$ depends on the mean fields.

If initially there are not excitations, i.e. the electromagnetic mode is in the vacuum state $|0\rangle$ and all the atoms are in their ground states, then the time evolution will be generated by the operator $H_{0,0}$ given in Eq. (160).

However, for parameters inside the white regions, the stationary point $\alpha = \beta = 0$ is unstable, and small perturbations in the mean fields are exponentially amplified in time.

If the mean fields have acquired macroscopic values, then, for a slow driving $\eta \ll \omega_a, \omega_b$, the trajectories lag behind one of the two broken symmetry points $(\alpha_\pm^{(sr)}, \beta_\pm^{(sr)})$ as μ get values smaller than one, as seen from the trajectories of the photon mean field α in Fig. 6.3.1 **(b)**-**(d)**, ($\beta(t)$ follows similar trajectories).

6.3.1 Photon Generation from the Vacuum and Work Done

The dynamic mean fields are not sufficient to obtain the average value of a generic observable.

In general, both the mean fields and the quantum fluctuations contribute to the evolution of the physical observable, and a complete quantum description requires the knowledge of the (operator) fluctuations around the mean fields.

The first moments of the quadratures are $\langle \hat{\boldsymbol{Q}}(t) \rangle$, while the second moments form the covariance matrix W with elements $W_{ij} = \langle \{\hat{Q}_i, \hat{Q}_j\} \rangle / 2 -$

$\langle\hat{Q}_i\rangle\langle\hat{Q}_j\rangle$ [139, 140, 134]. The covariance matrix at the time t is then given by $W(t) = \Phi(t)W(0)\Phi(t)^T$.

An interesting example being given by the average photon number $n_a = \langle\hat{a}^\dagger\hat{a}\rangle$, which reads

$$n_a = N\left|\alpha\right|^2 + \sqrt{2N}\left(\alpha_r\langle Q_1\rangle + \alpha_i\langle Q_3\rangle\right) + \left(W_{11} + W_{33} - 1\right)/2. \tag{170}$$

If initially the system is prepared in the state with no excitations, then $\alpha = \beta = 0\,\forall t$, so that photons are generated only by the exponential amplification of the initial fluctuations, due to the instability of the system under sinusoidal perturbation signalled by a positive instability rate γ^*.

For a very fast perturbation, $\eta \gg \omega_a, \omega_a\lambda_0$, this requires $\mu_0 < 1$, i.e. initially the system is in the SR region. On the other hand, if $\mu_0 > 1$, fluctuations are bounded in time. Differently, as the perturbation becomes slow, photon production can occur also if $\mu_0 > 1$, thanks to the Arnold instability tongues.

Photon generation from the vacuum is related to the work done on the system by the driving agent, that is

$$\begin{aligned} W_{done} &= \omega_a n_a(t) + N\omega_b(0)/2 + 2gW_{12}(t) \\ &\quad + \omega_b(t)\left[W_{22}(t) + W_{44}(t) - (N+1)\right]/2 \end{aligned} \tag{171}$$

and depends not only on the local energies of the two fluctuation modes involved, but also on their correlations through the W_{12} term.

Eq. (171) shows that not all of the energy pumped into the system is used for photon production: part of such energy goes to the atoms and part is stored as interaction energy.

The non-adiabaticity of the driving process can be quantitatively studied using the inner friction $[A]$, discussed in Sec. 3.2.

In our case, assuming the coupling to be switched on at $t = 0$, it reads $\langle w_{fric}\rangle = \langle w\rangle - E^t_{GS} + E^0_{GS}$, where E^t_{GS} is the energy of the instantaneous ground state of the system, which becomes non-analytic for $\mu = 1$.

The inner friction could get macroscopic values as the evolved state becomes macroscopically different from the instantaneous ground state. Altogether, the inner friction per atom in the thermodynamic limit is

$$\lim_{N\to\infty} \langle w_{fric}\rangle/N = \begin{cases} 0 & \text{for } \mu(t) \geq 1, \\ \omega_b(t)[1-1/\mu(t)]^2/4 & \text{for } \mu(t) < 1. \end{cases} \tag{172}$$

6.3.2 Characterization of the Fluctuations

Besides the mean photon number, we can characterize the photons generated by the variance $\sigma_a^2 = \langle (a^\dagger a)^2\rangle - n_a^2$, that reads

$$\sigma_a^2 = 2N\left(\alpha_r^2 W_{11} + \alpha_i^2 W_{33} + 2\alpha_r\alpha_i W_{13}\right) + \mathcal{O}(\sqrt{N}) \tag{173}$$

and, in the regime in which the mean fields dominate with respect to quantum fluctuations, we expect that the terms $\mathcal{O}(\sqrt{N})$ can be neglected for very large N.

A useful quantity characterizing the statistics of the photons is the Mandel parameter, that can be defined as $\rho = \frac{\sigma_a^2}{n_a}$. It signals a sub- or super-Poissonian statistics if ρ is less than or greater than one, respectively, with $\rho = 1$ for a coherent state, and $\rho = 0$ for photon number states.

For non zero mean fields, as $N \to \infty$, the Mandel parameter becomes

$$\rho_\infty = 2(\alpha_r^2 W_{11} + \alpha_i^2 W_{33} + 2\alpha_r\alpha_i W_{13})/|\alpha|^2 \tag{174}$$

In general terms, the time behavior of the quantum fluctuations is very different depending on wether μ is larger or smaller than 1. This is reflected in the covariance matrix and witnessed by the parameter ρ_∞ (see Fig. 6.3.2). Roughly, this is an oscillating function of time, which oscillates faster as the mean fields get larger, with an amplitude that suddenly increases whenever μ crosses one to enter in the SR region.

While n_a and ρ describe the reduced photon-state only, we can also characterize global state correlations by evaluating the degree of two-mode squeezing. With this aim, we consider the parameter $r_{opt}(t)$ optimizing the fidelity [141]

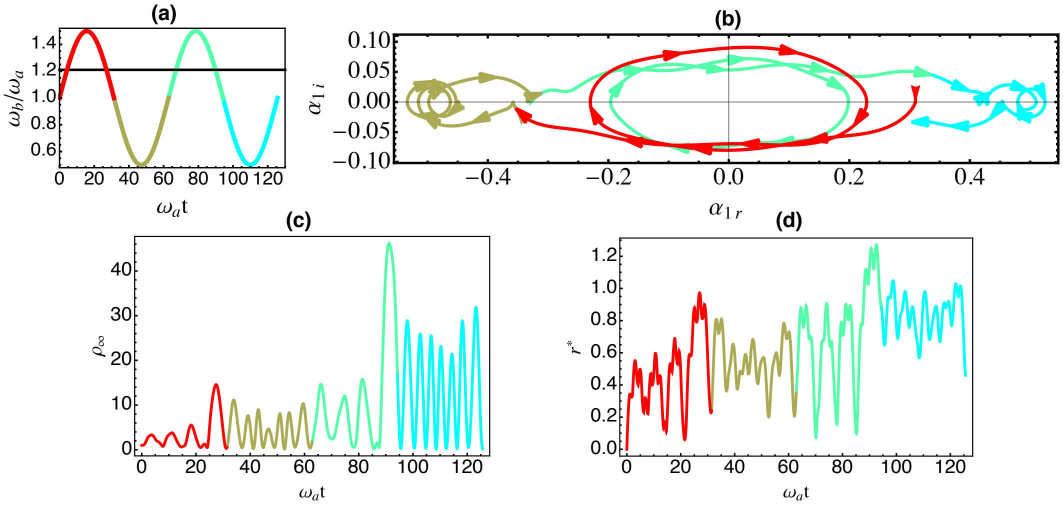

Figure 6.3.2.: (Color online): We show the driving cycle [panel **(a)**], the mean field trajectory **(b)**, the photon number fluctuations ρ_∞ **(c)**, and the two-mode squeezing parameter r^* **(d)**. In panels **(b)**-**(d)**, segments of a given color refer to the corresponding part of the driving cycle [panel **(a)**]. We set $\eta = 0.1\omega_a$ and $\lambda = 0.5$, with $\lambda_0 = 1$, and $g = 0.55\omega_a$. Initial conditions are $\alpha(0) = \alpha^{(sr)}(0)$ and $\beta(0) = \beta^{(sr)}(0)$.

between $|\psi, t\rangle$ and the two-mode squeezed coherent state [134] $\left|\psi_{\alpha,\beta}(r,t)\right\rangle$ having coherent amplitudes given by the mean fields and (real) squeezing degree r, i.e. $|\psi_{\alpha,\beta}(r,t)\rangle = e^{r(c^\dagger d^\dagger - cd)} |\alpha(t)\rangle_a |\beta(t)\rangle_b$. Regardless of t, we numerically find a value $r_{opt}(t)$ for which the fidelity is ≥ 0.9999. Therefore, r_{opt} itself can be thought as a good (although approximate) descriptor of the photon-atom entanglement, [142, 133]. During time evolution, it turns out that r_{opt} can either grow exponentially at short times (if $\gamma^* > 0$), or remain very close to its initial value (for $\gamma^* = 0$). An example of the behavior of r_{opt} is reported in Fig. (6.3.2), for the various stages of the driving induced dynamics.

6.4 SUMMARY AND CONCLUSIONS

In this Chapter, we have considered an out of equilibrium process generated by parametrically driving the Dicke model. The study has been done for an arbitrary driving, and the system has been described in terms of two classical mean fields, by taking into account also the quantum fluctuations around them. Depending on the driving, the quantum fluctuations (and also the mean fields) could experience an unbounded amplification in time, that should be attributed to a quantum dynamical phase transition.

The analysis is carried on by mainly focusing on a periodic driving, that could generate a parametric amplification of the vacuum fluctuations. This mechanism, mimicking the Dynamical Casimir effect, is linked to the thermodynamic work done in the process. Furthermore, the non adiabaticity of the evolution is characterized in terms of the inner friction. The quantum fluctuations, described by the covariance matrix, are also characterized in terms of some figures of merit, which are the Mandel parameter and the degree of two-modes squeezing.

CONCLUSIONS

In this Thesis we have reported the doctoral studies performed in the last three years. These studies are rooted in the field of the quantum thermodynamics, and the paradigm of the work fuctuations theorems, discussed in Chap. 2, has been like a germ, from which the most part of the results presented here have developed. In this scenario, a physical system is driven far from an initial equilibrium state by changing some Hamiltonian parameters. We have carried out a general theoretical analysis, described in Chap. 3, by considering two hypothetical reference processes, an isothermal and an adiabatic reversible transformation. The latter has permitted to define the so-called quantum inner friction, that has been linked to a Tasaki fluctuation relation.

Such general formalism has been briefly illustred with the help of two paradigmatic examples, which are a harmonic oscillator and a spin 1/2.

An entropic measure of non adiabaticity, that in special circumstances could be identified with the inner friction, is also introduced and discussed from a thermodynamic point of view.

Specifically, it has been related to the work done in the process, and studied as the process tends to be adiabatic, finding an interesting relation involving the relative entropy of coherence. The role of the quantum coherence is still object of our investigations, however some general relations, employing such coherence measure, have beem reported in Chap. 3.

The tools underlying this general framework have been used in the characterization of out of equilibrium processes in specific many-body systems. We have considered a quantum Ising spin (open) chain in a transverse field, abruptly brought out of equilibrium because of a sudden quench, localized on its boundary (Chap. 5). The system has been studied thanks to a fermionic representation, and the non-equilibrium thermodynamics has been characterized, by looking on the statistics of the work done in this process, which shows a signature of the quantum phase transition of the system. The system is linked to a Kitaev chain, and in order to fully understand the role played by the Majorana zero mode, we have also examined the out of equilibrium dynamics generated by the quench. This has been characterized by focusing on the propagation of the magnetization disturbance along the chain, finding strong oscillations in the transient regime as the Majorana zero mode is involved.

Another critical model is considered in Chap. 6, namely the Dicke model. The out of equilibrium process is discussed for an arbitrary driving. Technically, our analysis has been mostly focused on the thermodynamic limit, and has been based on two macroscopic mean fields and the quantum fluctuations around them. In particular, the circumstances under which the quantum fluctuations become unbounded in time have been discussed in general, and characterized in the case of a periodic driving. A generation of photons from the vacuum state could occur because of a parametric amplification of the quantum fluctuations. This mechanism, mimicking the Dynamical Casimir effect, has been linked to the non equilibrium thermodynamics, by characterizing the work done.

The problem of work extraction in finite quantum systems has been also considered in general in Chap. 4. There, a new procedure of work extraction, employing the quantum correlations between the system and an ancilla, has been introduced and deeply studied. The amount of work extracted can be enhanced, thanks to the information on the state of the system acquired from measurements on the state of the ancilla. The maximum gain in work (daemonic gain) acts as witness for the quantum correlations embodied by the quantum discord, and as a necessary and sufficient criterion of separability of bipartite pure states. Our analysis has been carried out by considering an illustrative example of two qubits, for which we have fully characterized the distribution of quantum correlated states with respect to the figure of merit set by the daemonic ergotropy, finding that quantum correlations embody a proper resource for the work-extraction performances of the states that minimize the daemonic gain.

LIST OF PUBLICATIONS

[*A*] F. Plastina, A. Alecce, T. J. G. Apollaro, G. Falcone, G. Francica, F. Galve, N. Lo Gullo, and R. Zambrini. Irreversible Work and Inner Friction in Quantum Thermodynamic Processes. *Phys. Rev. Lett.*, 113:260601, 2014.

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[*C*] G. Francica, T. J. G. Apollaro, N. Lo Gullo, and F. Plastina. Local quench, Majorana zero modes, and disturbance propagation in the Ising chain. *Phys. Rev. B*, 94:245103, 2016.

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[*E*] G. Francica, J. Goold, M. Paternostro and F. Plastina. Daemonic Ergotropy: Enhanced Work Extraction from Quantum Correlations. arXiv:1608.00124v1 (accepted for publication by Nature NPJ Quantum Information), 2016.

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