Equilibration and thermodynamics of quantum systems

by

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supervised by

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Abstract

In this thesis we study two topics topics within quantum statistical mechanics and quantum thermodynamics: the equilibration time scales of quantum systems, and the process of work extraction from quantum systems.

After introducing the notion of equilibration of quantum systems in Chapter 2, and proving a general upper bound on the equilibration time scales for any observable, we show in Chapter 3 the existence of both observables with extremely slow and extremely rapid equilibration. Interestingly, we find that the typical behaviour of a set of observables initially out of equilibrium turns out to give rapid time scales as well.

In Chapter 4 we address the problem of understanding, from first principles, the conditions under which a closed quantum system equilibrates within physically realistic times with respect to a given observable. We provide an upper bound on the equilibration time scales which, under some physically reasonable conditions, shows that equilibration may be in fact mush faster than the extremely slow cases found in Chapter 3. In particular, we apply this result to give bounds on the time scales of equilibration for a system interacting with a bath which, unlike previously known general upper bounds, do not scale with the size of the bath.

On Chapter 5 we introduce the topic of thermodynamic work extraction from quantum systems, from the perspective of treating non-thermal states as a resource. We then extend this approach to account for the fact that quantum operations which do not commute with the total energy also constitute a potentially valuable resource.

Dedication

To Faustina, on your birthday.

Acknowledgements

I would like to start by thanking those who made this PhD thesis possible in the first place: my supervisors Andreas Winter and Noah Linden. Andreas is responsible for me coming to Bristol, and has been extremely supportive from day one. Once Andreas left to Barcelona, Noah become the person I would turn to for advice in Bristol, and his guidance has marked my PhD. I am forever grateful to both of them. A line goes to my PhD examiners Toni Acín and Sandu Popescu, for taking the time to read this thesis and the very interesting discussion during the viva.

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If at any point perseverance eluded me, thinking of Abue immediately refreshed it; her strength is an immense source of inspiration, and I thank her for that. On crucial stages of my life, my mind invariable remembers those who I miss the most: Dorita de Arteaga, Alberto

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[1] I also give her credit for some of the artwork in this thesis, in particular Figure 1.1.

Declaration

I declare that the work in this dissertation was carried out in accordance with the requirements of the University's Regulations and Code of Practice for Research Degree Programmes and that it has not been submitted for any other academic award. Except where indicated by specific reference in the text, the work is the candidate's own work. Work done in collaboration with, or with the assistance of, others, is indicated as such. Any views expressed in the dissertation are those of the author.

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Contents

Chapter 1

Preface

1.1 Classical and quantum thermodynamics

Classical thermodynamics, one of the pillars of classical physics, addresses the behaviour of macroscopic systems in thermodynamical equilibrium, that is, systems for which their macroscopic properties (e.g. energy, temperature, chemical potential) remain constant. This theory arose from experimental observation, which led to the formulation of a series of laws that can be expressed as follows.

- Zeroth law: Two systems in thermal equilibrium with a third one are also in equilibrium with each other.
- First law: Energy is constant in a closed system.
- Second law (Kelvin statement): No thermodynamic process exists which can solely extract heat from a bath and transform it entirely into work.
- Third law: The entropy of a system at zero temperature is zero.

In combination with an equation of state, these laws allow defining and relating the relevant physical quantities necessary in order to explain the general properties and allowed transitions of thermodynamic systems. For instance, the zeroth law helps to define temperature, as the property shared by any two systems in thermal equilibrium, while the third law serves to uniquely determine entropy. Within the processes that satisfy the first law, the second law defines those that are physically possible in thermodynamic transitions. This deeper law forbids processes that are not observed in nature for macroscopic systems, like a

cup of coffee increasing temperature by spontaneously absorbing heat from its surrounding air. For an introduction to classical thermodynamics see [1].

Remarkably, the combination of these phenomenological laws and experimentally inspired concepts gave a framework from which a myriad of practical applications where obtained. Historically notable for modern society was, for instance, the quest for more efficient steam engines during the first half of the 19th century. In general, as experimental capabilities increased, physicists have been able to address and probe much smaller systems, where quantum mechanics begins to play a preponderant role. Therefore, it is not surprising that in the past decades there has been considerable theoretical and experimental effort dedicated to extending thermodynamics into the quantum realm, and testing its validity in this regime.

One example of such endeavor to extend thermodynamics to the quantum regime deals with quantum refrigeration, i.e. the process of cooling of quantum systems, which was studied in [2–4], with a minimalist model of a quantum refrigerator consisting of two qubits considered in [5]. Another one is Maxwell's demon, who claims he is able to extract work from heat in a cyclic process [6, 7], and was proven to be cheating by Landauer's erasure principle, which states that heat is produced in order to reset the demon's memory [8]. These deep concepts connecting information theory and thermodynamics where analysed from a quantum mechanics perspective in [9, 10].

Moreover, the laws of thermodynamics themselves have been cause for much attention. The zeroth law, along with the conditions under which temperature can be proven to be a local property, was investigated in [11–13], while [14] deals with deriving the third law from first principles in the quantum regime (for more thorough presentations on quantum thermodynamics the reader is encouraged go to the recent reviews [15, 16]), or the textbook by Gemmer, Michel, and Mahler [17].

Given its practical relevance, substantial effort has been dedicated to the second law and the related limits on work extraction from quantum systems [18–24], and even to debating on the notion of work itself in the quantum regime [25, 26], or on the connection between coherence in the energy basis (a purely quantum concept) and work extraction [27–30]. We will address the topic of work extraction in Chapter 5 of this thesis, overviewing it in the classical and quantum regimes. Furthermore, in Section 5.3 we introduce the idea of

extracting work out of a system undergoing a quantum evolution that does not naturally arise from the interaction with systems in thermal states, i.e., work extraction from non-thermal channels.

1.2 Classical and quantum statistical mechanics

Statistical mechanics emerged as a means to understand at a deeper level how the phenomenological concepts introduced by thermodynamics arise. This theory is conceptually grounded on the idea that, in order to describe the general behaviour of, for example, a gas, the particular movements of each molecule is not relevant. In other words, the thermodynamical properties of macroscopic systems can be explained without the need to address the behaviour of its microscopic constituents.

This simple notion motivates the following fundamental hypothesis behind statistical mechanics, which we illustrate in Figure 1.1.

Assumption 1.1 (Equal a priori probabilities)**.** *For a closed system with some given physical constrains (i.e. in a state with a given energy, number of particles, volume, etc.), the system can be found in any compatible microstate with the same probability.*

On these grounds, the microcanonical ensemble comes naturally as the statistical ensemble consisting of all microstates with equal probabilities in the above assumption. Moreover, if the interaction between some small system and an environment is weak, assuming the microcanonical ensemble for system and bath leads to the canonical ensemble.

As Boltzmann insightfully discovered, the number of accessible microstates Ω is related to the thermodynamical entropy S via the following equation

$$S = K_B \ln(\Omega), \tag{1.1}$$

where K_B is Boltzmann's constant.

This equation connects the purely statistical mechanical quantity Ω to a fundamental physical quantity in the field of thermodynamics, the entropy S. In this way, it provides us with a deeper physical understanding of the concept of entropy as quantifying our lack of knowledge of the system's microstate, otherwise phenomenologically defined. This serves as

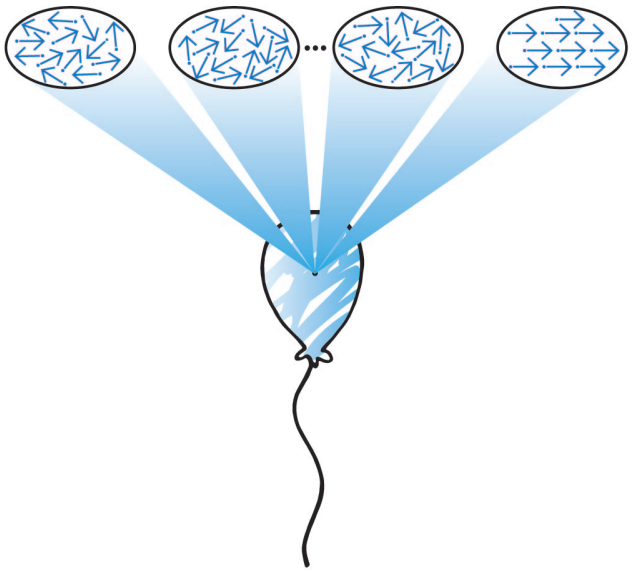

Figure 1.1: Illustration of the equal a priori probabilities postulate. All microstates of the gas inside the balloon compatible with a given energy, volume, and number of particles are assumed to have the same probability. Even though some accessible microstates, like the one depicted on the upper right, correspond to a non equilibrium situation, the vast majority of them correspond to one (equilibrium) macrostate, which "explains" why we observe the balloon in equilibrium for most of the times.

starting point for statistical mechanics as a basis for the theory of thermodynamics. For a more thorough treatment of statistical mechanics and its relationship with thermodynamics see for example [31].

Given that statistical mechanics refers to the microscopic constituents that make up macroscopic bodies, it has naturally not been foreign to quantum theory from its beginnings. Nevertheless, a modern development which illustrates how quantum theory can shed light into the foundations of statistical mechanics has sparked considerable work on quantum statistical mechanics.

Popescu, Short, and Winter studied whether the equal a priori probabilities postulate can be understood on a quantum mechanical basis. Let us briefly review the main ideas behind their result. Consider a small system $\mathcal{S}$ and an environment $\mathcal{E}$, and assume the composite system $\mathcal{S}+\mathcal{E}$ is in a pure state Ψ, belonging to a Hilbert space $\mathcal{H}_R$. This space is assumed to be defined such that the states it contains satisfy the constraints of some given macrostate (for example, a given energy or number of particles).

The state of the small system $\mathcal{S}$ is given by the reduced density matrix obtained after tracing out the environment,

$$\rho_S = \mathrm{Tr}_{\mathcal{E}} \left[|\Psi\rangle \langle\Psi| \right]. \tag{1.2}$$

The authors showed that for most states $|\Psi\rangle$ this reduced density matrix is close to [1] the state $\frac{1}{d_R} \mathrm{Tr}_{\mathcal{E}} [\mathbb{1}_{\mathcal{H}_R}]$, where $\mathbb{1}_{\mathcal{H}_R}$ is the identity on $\mathcal{H}_R$ and $d_R = \mathrm{Tr}[\mathbb{1}_{\mathcal{H}_R}]$. Notice that the state $\frac{\mathbb{1}_{\mathcal{H}_R}}{d_R}$ assigns equal probabilities to any possible microstate within the space with the considered constraints; it is exactly the state corresponding to the microcanoncial ensemble [32]. Hence, the authors found that for most $|\Psi\rangle$ the state of any small subsystem is *as if* the equal a priori probabilities holds, and in doing so they found a way to understand how probabilities can arise in statistical mechanics even if the actual state of the universe was exactly known. Notably, Lloyd had considered ideas along this same line in his PhD thesis, see Ref. [33], and Goldstein, Lebowitz, Tumulka, and Zanghì in [34], which they traced back to Schrödinger.

Once the microcanonical ensemble is motivated by the above considerations, as in the classical case it can be assumed as starting ground to prove the canonical one [35–38]. These results are deeply related to the way in which thermal states arise in quantum statistical mechanics, known as the problem of thermalization, an interesting topic which is seeing advances [39–47].

The equal a priori probabilities postulate in classical statistical mechanics can also help picture why thermodynamic systems are typically found in equilibrium, even when their microscopic constituents are continually evolving. Since the vast majority of microstates correspond to one equilibrium macrostate, it is overwhelmingly more likely to find the system in thermodynamic equilibrium than out of it. One could even argue that this same reason is behind the rapid approach to equilibrium that is typically observed in nature. This question was also addressed by Boltzmann in what is referred to as the H-Theorem [48, 49], with various criticisms at the time, notably by Loschmidt [50] and Zermelo [51]. However, Boltzmann's result is based on a particular model and several assumption, so it does not constitute a satisfactory proof of how out of equilibrium situations dynamically evolve to equilibrium in general (for a modern overview on Boltzmann's approach, and a discussion of

[1] We will define distance between quantum states in Chapter 2, but at this point it is enough to mention that by closeness we refer to the fact that both states lead to similar experimental observations.

the criticisms, see [52]).

In Chapter 2 of this thesis we will review in detail the conditions that allow proving that systems approach equilibrium, and the possible ways in which equilibrium can be defined in quantum mechanics, which has attracted great attention in the past decades [53–58]. In turn, Chapters 3 and 4 will be devoted to the time scales involved in the equilibration process, a topic which, given its complexity, had seen less breakthroughs than the other ones mentioned here, some of which are [59–63].

Many of the topics considered above, for which we have included a series of recent references, actually go back to the founding fathers of quantum mechanics, most notably von Neumann and Schrödinger [48, 49, 64, 65]. For more thorough treatments of topics within quantum statistical mechanics the reader can recur to the reviews [66, 67].

1.3 Outline of the thesis

We start in Chapter 2 with an overview of previous results on the equilibration of closed quantum systems, which will serve as introduction for the two following chapters. After explaining two alternative and complementary concepts of equilibration, namely equilibration of small systems interacting with an environment and equilibration of systems with respect to observables, we introduce general conditions which ensure equilibration occurs. We end by presenting some general results on equilibration in finite time which provide upper bounds on the time scales of equilibration for any observable. This chapter is mainly reviews the leading work by Reimann [53], Linden, Short, Popescu, and Winter [54], and Short and Farrelly [59].

Chapter 3 is devoted to investigating the possible extremes of the equilibration time scales. Here we show how to construct both observables with extremely slow and observables with extremely rapid equilibration. This chapter is based on joint work with Artur Malabarba, Noah Linden, Terrence Farrelly, and Anthony Short, and has been previously published as "Quantum Systems Equilibrate Rapidly for Most Observables", Phys. Rev. E **90**, 012121 (2014) [68].

In Chapter 4 we turn to the search of observables which, unlike the ones constructed in Chapter 3, equilibrate in physically realistic time scales. By the end of this quest we are left with a set of conditions which ensure that the observable considered does not fall within

the ones with extreme time scales. This chapter is based on joint work with Noah Linden, Artur Malabarba, Anthony Short, and Andreas Winter, and is available as the preprint "Equilibration time scales of physically relevant observables", arXiv:1509.05732 [69].

Chapter 5 starts with an introduction to work extraction, first in classical thermodynamics and then in quantum thermodynamics. In the latter, we emphasize the resource theory approach to quantum thermodynamics, wherein non-thermal states are viewed as a resource from which work can be extracted. This serves as motivation for studying, in Section 5.3, a complementary viewpoint in which non-thermal channels are taken as a resource. This is based on joint work with Miguel Navascués, and has previously been published as "Non-thermal quantum channels as a thermodynamical resource", Physical Review Letters **115**, 010405 (2015) [70].

In order to keep the flow of the text, we devote Appendix A to some lengthier calculations.

Chapter 2

Introduction to the equilibration of closed quantum systems

This chapter presents an overview of previous work on the equilibration of closed quantum systems, which will serve as introduction for the two following chapters. After general considerations on the equilibration of closed systems, we explain in Section 2.1 the concept of state equilibration, and show general conditions which allow proving that the state of any small subsystem of a large system equilibrates. Section 2.2 is devoted to the complementary approach of observable equilibration, where the focus is on the evolution of concrete observables. We end in Section 2.3 with general results on the time scales involved in the equilibration process, and in particular with a general upper bound on the equilibration time scale valid for any observable.

Let us consider a system with a Hamiltonian H, a d dimensional Hilbert space $\mathcal{H}$, and an initial state given by the density matrix $\rho_0 \in \mathcal{H}$. At a later time t the system evolves according to

$$\rho_t = e^{-iHt}\rho_0 e^{iHt}, \tag{2.1}$$

where we assume units in which $\hbar = 1$.

The state's evolution is, formally, extremely simple. If we denote the eigenvalues and eigenvectors of H by E_j and $|j\rangle$ respectively, a pure initial state can be written as

$$\rho_0 = \sum_{j,k=1}^{d} c_j c_k^* \left|j\right\rangle \left\langle k\right|, \tag{2.2}$$

where the complex coefficients c_j satisfy $\sum_{j=1}^{d} |c_j|^2 = 1$. The evolved state is then given by

$$\rho_t = \sum_{j,k=1}^{d} c_j c_k^* e^{-i(E_j - E_k)t} |j\rangle \langle k| . \tag{2.3}$$

Notice that, for simplicity, we focus on pure initial states, but it is simple to extend the results to mixed initial states by purification [56].

Now we ask whether the system's natural evolution leads, in some sense that we will specify, to a quasi-static situation. We refer to this as the *problem of equilibration*.

In order to address this topic we start by considering some figure of merit to quantify distance between states, i.e., some quantity which at time t tells us how far the system is from the static, equilibrium, situation. Let us assume that this equilibrium situation is represented by some state ω, and denote the quantifier of distance between ρ_t and ω by $\mathcal{D}_*(\rho_t, \omega)$. The distance is assumed to be positive, and that it becomes smaller as the instantaneous state approaches the equilibrium one. Later on we will show examples of different distances $\mathcal{D}_*$, and their respective meanings (the trace distance is one such possibility, but as we will see other possibilities are often more relevant).

We emphasize that we will not be concerned with the details of the equilibrium state ω, and in particular this state need not be thermal. Proving the conditions under which ω is thermal, a very interesting problem in itself, is referred to as the *problem of thermalization*, as mentioned in the introduction, and is beyond the scope of this thesis.

In finite dimensional systems the evolution is characterized by a finite number of Bohr frequencies $(E_j - E_k)$, as can be seen from eq. (2.3). This implies that there always exist revivals, or recurrences, in the evolution. That is, there exists a time τ_{rec} at which the state is arbitrarily close to the initial state [71], $\rho_{\tau_{\text{rec}}} \approx \rho_0$, analogous to Poincaré recurrences in classical systems. Therefore, for any distance $\mathcal{D}_*$ that we choose, we have

$$\mathcal{D}_*(\rho_0, \omega) \approx \mathcal{D}_*(\rho_{\tau_{\text{rec}}}, \omega). \tag{2.4}$$

This excludes the possibility that the system stays close to equilibrium for all times after some time t_{eq}; *equilibration cannot occur in a strict sense*. See Figure 2.1 for an illustration.

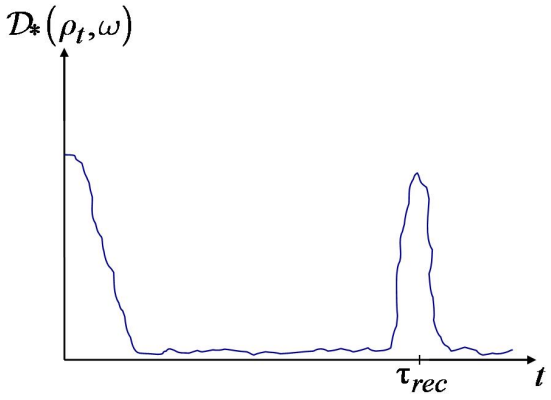

Figure 2.1: Illustration of a revival in the evolution. After a time τ_{rec}, in general very long [72], the state $\rho_{\tau_{\text{rec}}}$ comes close to the initial state ρ_0. This is manifested in any distance $\mathcal{D}_*$.

Therefore, we have to consider a notion of equilibration which can account for this, and incorporates deviations out of equilibrium. One such possibility, the one we will adopt in this thesis, is the idea of *equilibration in average*: does the system spend *most* of its time close to equilibrium?

Denoting the time average by $\langle f(t)\rangle_T \equiv \frac{1}{T}\int_0^T f(t)dt$, we define equilibration as follows.

Definition 2.1 (Equilibration)**.** *A system equilibrates to the state ω with respect to the distance $\mathcal{D}_*$ and the equilibration constant χ when*

$$\langle \mathcal{D}_*(\rho_t,\omega)\rangle_\infty \leq \chi, \tag{2.5}$$

where $\langle f(t)\rangle_\infty \equiv \lim_{T\to\infty}\langle f(t)\rangle_T$.

This definition, which depends on the value of χ that one chooses, is most significant for $\chi \ll 1$. Since in such a case the infinite time average is small, and due to the fact that the distance $\mathcal{D}_*$ is positive, for most times along the system's evolution the instantaneous distance $\mathcal{D}_*(\rho_t,\omega)$ must be small. In more precise terms, eq. (2.5) bounds the fraction of times the system spends out of equilibrium, as measured by $\mathcal{D}_*$. Indeed, the fraction of times for which $\mathcal{D}_*(\rho_t,\omega) \geq \chi K$ is smaller than $\frac{1}{K}$.

These general ideas can be formalised in different ways depending on the definition used for the distance $\mathcal{D}_*$, each implying a different notion of equilibration. In the next two

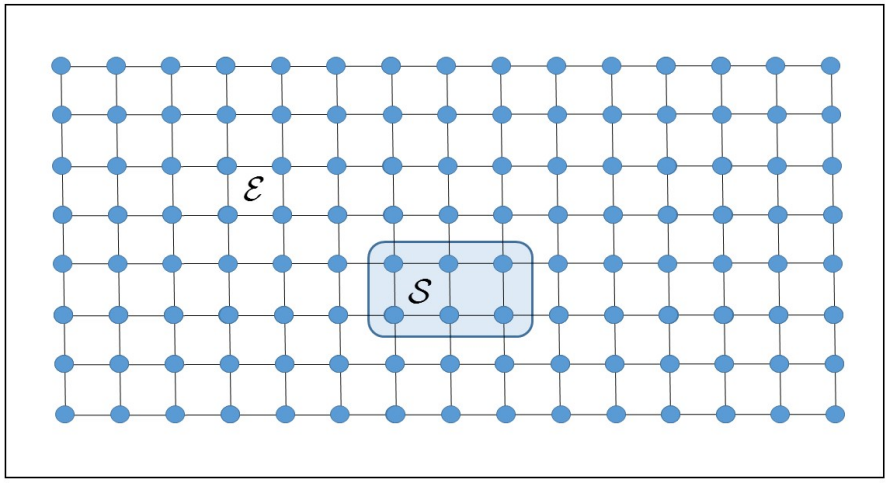

Figure 2.2: Illustration of an environment $\mathcal{E}$ interacting with the system $\mathcal{S}$. In the picture the system $\mathcal{S}$ is taken as a subsystem of a larger, closed, system, while the remainder is the environment $\mathcal{E}$. The links represent interactions between the constituent entities that make up the whole system plus environment.

sections we will introduce two alternative notions, that of state equilibration and of observable equilibration.

2.1 State equilibration

In practice systems are not isolated. Hence, a very natural question to ask is what the dynamics of a system $\mathcal{S}$ in contact with a second (in general larger) one are. We call this second system the *environment*, and denote it by $\mathcal{E}$ (see Figure 2.2 for an illustration). We denote the Hilbert spaces associated to system and environment by $\mathcal{H}_\mathcal{S}$ and $\mathcal{H}_\mathcal{E}$ respectively.

In general the system always interacts, at least weakly, with systems farther and farther away, in an infinite, intractable, chain. However, in practice one can define the environment as the composition of the systems that most strongly interact with $\mathcal{S}$, and disregard the rest of the infinite chain. In such a case, the system plus relevant environment can be taken as one closed system. The evolution is then given by eq. (2.3) on page 10.

The question that we address in this section is whether the system, due to the interaction

with the environment, equilibrates.

If the density matrix ρ_t acting on $\mathcal{H}_\mathcal{S} \otimes \mathcal{H}_\mathcal{E}$ represents the state of the system plus environment, the state of the system at time t is given by the reduced density matrix $\rho_t^\mathcal{S}$ on $\mathcal{H}_\mathcal{S}$ obtained after tracing out the environment,

$$\rho_t^\mathcal{S} = \mathrm{Tr}_\mathcal{E}\left[\rho_t\right]. \tag{2.6}$$

Likewise, if ω is the state representing the equilibrium situation, when tracing out the environment we get

$$\omega^\mathcal{S} = \mathrm{Tr}_\mathcal{E}\left[\omega\right], \tag{2.7}$$

which represents the equilibrium state for the system $\mathcal{S}$.

Now we define a distance between states. One natural distance between density matrices comes from considering the trace norm, defined for an operator A as

$$\|A\|_1 \equiv \mathrm{Tr}\left[\sqrt{A^\dagger A}\right]. \tag{2.8}$$

If A is an Hermitian operator with eigenvalues λ_j this becomes $\|A\|_1 = \sum_j |\lambda_j|$. For an introduction to matrix norms and many of the properties that will be used in this thesis see [73], or the lecture notes [74].

The *trace distance* is then defined as follows.

Definition 2.2 (Trace distance)**.** *For two states σ_1 and σ_2,*

$$\mathcal{D}(\sigma_1, \sigma_2) \equiv \frac{1}{2}\|\sigma_1 - \sigma_2\|_1. \tag{2.9}$$

This distance has a very physical interpretation: it quantifies how distinguishable both states are via *any possible measurement*. More precisely, one can see that

$$\mathcal{D}(\sigma_1, \sigma_2) = \max_P \mathrm{Tr}\left[P\left(\sigma_1 - \sigma_2\right)\right], \tag{2.10}$$

where the maximization is over all projectors P. Hence, the trace distance tells us by how far the probability of any measurement can differ for the two states (see Section 9.2 of [75]). If

$\mathcal{D}(\sigma_1, \sigma_2) = 1$, then there exists *some* measurement P which perfectly discriminates the two states. On the other hand, if $\mathcal{D}(\sigma_1, \sigma_2) = 0$ then the states are the same $\sigma_1 = \sigma_2$. Moreover, the probability of successfully guessing between states σ_1 and σ_2 via any measurement, assuming both are given with equal probability, satisfies $p_{\text{success}} = \frac{1}{2}\left(1 + \mathcal{D}\left(\sigma_1, \sigma_2\right)\right)$.

With these tools, Linden, Popescu, Short, and Winter studied in detail the problem of state equilibration in [54]. In the paper they proved equilibration by assuming the following.

Assumption 2.3 (Non-degenerate energy gaps)**.** *A Hamiltonian has no degenerate energy gaps if the energy difference of any two pairs of distinct energy levels are different.*

With this assumption, they proved that for a pure initial state ρ_0,

$$\left\langle \mathcal{D}\left(\rho_t^{\mathcal{S}}, \omega^{\mathcal{S}}\right) \right\rangle_\infty \leq \frac{1}{2}\sqrt{\frac{d_S^2}{d_{\text{eff}}}}, \tag{2.11}$$

where d_S is the dimension of $\mathcal{H}_{\mathcal{S}}$, and the equilibrium state is $\omega^{\mathcal{S}} = \text{Tr}_S\left[\omega\right]$ with $\omega \equiv \left\langle \rho_t \right\rangle_\infty$.

Due to the non-degenerate gaps assumption, the infinite time averaging destroys all off diagonal terms in the instantaneous state in eq. (2.3) on page 10, and

$$\omega = \lim_{T\to\infty} \frac{1}{T}\int_0^T \rho_t dt = \sum_{j=1}^{d} |c_j|^2 \left|j\right\rangle \left\langle j\right|. \tag{2.12}$$

The *effective dimension* d_{eff} is defined as follows.

Definition 2.4 (Effective dimension)**.** *Given an initial state ρ_0 with support on d_E distinct energy levels, and projectors P_j onto the distinct energies,*

$$d_{\text{eff}} \equiv \frac{1}{\sum_{j=1}^{d_E}\left(\text{Tr}\left[\rho_0 P_j\right]\right)^2}. \tag{2.13}$$

For pure states this becomes $d_{\text{eff}} = \frac{1}{\sum_{j=1}^{d_E}|c_j|^2}$. The effective dimension quantifies how spread the state is among different energy levels. For instance, if only one energy level is populated $d_{\text{eff}} = 1$, while on the other hand, if one has an equal superposition of d_E levels then $d_{\text{eff}} = d_E$. Therefore, d_{eff} gives an idea of how many energy levels are populated in the state, and their respective weights.

Equation (2.11) implies that, whenever the dimension of the system $\mathcal{S}$ is small compared to $\sqrt{d_{\text{eff}}}$, the system's state will be close to the time averaged state for most times $t > 0$, i.e. the system equilibrates according to Definition 2.1 on page 11.

In general one expects this to hold whenever a small system $\mathcal{S}$ interacts with a large environment $\mathcal{E}$, since in such a case many energy levels tend to be populated, implying a high effective dimension. One way to picture this is to consider an environment composed of many constituents; for instance, let $\mathcal{S}$ be a spin and $\mathcal{E}$ a collection of L spins. As the size of the environment increases, the energy window on which the state is supported increases as well. Typically this increase is proportional to $\sqrt{L}$, which can be seen by noting that the energy standard deviation, characterising the state's energy range, grows with $\sqrt{L}$. On the other hand, the dimension of the Hilbert space grows exponentially with the number of constituents, $d \sim e^{cL} d_S$. If the energy levels that appear as the size of the environment increases are all being populated, which seems expectable, we arrive at $d_{\text{eff}} \sim e^{cL} d_S$. Since the dimension of the system is kept fixed, for large environment we conclude that the right hand side of eq. (2.11) scales like $\sqrt{\frac{d_S^2}{d_{\text{eff}}}} \sim \sqrt{\frac{d_S}{e^{cL}}} \ll 1$.

In the paper Linden, Popescu, Short, and Winter mathematically supported this idea by studying what *typically* happens when the initial state is drawn uniformly at random from a given Hilbert space (more precisely, drawn at random from the Haar measure [76]). They found that, with high probability, the effective dimension is indeed extremely large. More precisely, when the state $|\psi\rangle$ is taken at random from a restricted space $\mathcal{H}_{\mathcal{R}} \in \mathcal{H}_{\mathcal{S}} \otimes \mathcal{H}_{\mathcal{B}}$ of dimension d_R the probability that $d_{\text{eff}} < d_R/4$ satisfies

$$\Pr\{d_{\text{eff}} < d_R/4\}_\psi \leq 2 \exp\Big(- c\sqrt{d_R}\Big), \tag{2.14}$$

where $c \approx 10^{-4}$. The restricted space accounts for possible physical constraints on the states considered (for example, a given number of particles or energy range). Hence, in the sense explained above, the probability of having a small effective dimension is exponentially small in the relevant Hilbert space dimension.

Let us consider more closely the conditions behind eq. (2.11). Firstly, the result might at first sight seem too general. What about those situations that we know do not lead to equilibration? For instance, in the case of a small system that does not interact with an

environment, with a Hamiltonian of the form $H = H_{\mathcal{S}} + H_{\mathcal{E}}$, there is no reason for the system to equilibrate. These Hamiltonians are ruled out by the non-degenerate energy gaps Assumption 2.3. We can easily check this by writing the eigenvectors of the system and environment Hamiltonian as $|s\rangle$ and $|e\rangle$ respectively, and noting that in this case the energy gap corresponding to the pair of levels $\{|s\rangle|e\rangle, |s\rangle|e'\rangle\}$ is identical to the energy gap of the pair of levels $\{|s'\rangle|e\rangle, |s'\rangle|e'\rangle\}$.

In general, both the non-degenerate gaps assumption and the high effective dimension condition, necessary to prove equilibration in this setting, provide some physical intuition. For example, consider an initial state in which only a few energies are populated, i.e. a situation with a low effective dimension. In this case the evolved state, given by eq. (2.3) on page 10, involves oscillations with only a few frequencies. It is hard to imagine how this would lead to a static situation; in fact, revivals would occur after short periods of time. A high effective dimension rules this out, by ensuring that many different energies, and therefore frequencies, are involved in the evolution. On the other hand, if an energy gap is extremely degenerate, as in the example of a non interacting system and environment in the previous paragraph, the frequency corresponding to this gap tends to dominate the evolution. Both conditions play the similar role of ensuring that there is a wide spectrum of frequencies involved in the evolution. The complex interplay of a vast number of different frequencies facilitates a situation in which the evolution leads to a quasi-static situation.

2.2 Observable equilibration

The trace distance is an extremely demanding notion of distance, which, as explained after Definition 2.2 on page 13, requires that equilibration occurs with respect to *every* mathematically conceivable observable (i.e. every Hermitian operator). Under this strict distance between states it is necessary to restrict to a system interacting with an environment in order to prove equilibration, as we saw on the previous section. However, when considered in its whole a closed system cannot equilibrate with respect to the trace distance. Indeed, since the trace norm is invariant under global unitaries, it does not change in time, so $\|\rho_t - \omega\|_1 = \|\rho_0 - \omega\|_1$, which implies that if the system starts out of equilibrium it will remain out of it.

Nevertheless, in practice physical observations are constrained to only a subset of all possible measurements. This fact motivates an alternative viewpoint on the equilibration problem that focuses on whether the system approaches equilibrium with respect to a concrete physical observable, represented by a Hermitian operator A.

Let us start by considering the equilibration of expectation values. That is, we focus on whether the instantaneous expectation value $\mathrm{Tr}\left[\rho_t A\right]$ approaches some equilibrium value $\mathrm{Tr}\left[\omega A\right]$, and remains close to it for most times. Here, and from now on, ω is the steady state density matrix that characterizes the equilibrium situation.

Consequently, we define the *weak-distinguishability* as a measure of distance, as follows.

Definition 2.5 (Weak-distinguishability)**.** *For an observable A and any two states σ_1 and σ_2, the weak-distinguishability is*

$$\widetilde{\mathcal{D}}_A\left(\sigma_1,\sigma_2\right) \equiv \frac{\left|\,\mathrm{Tr}\left[\sigma_1 A\right] - \mathrm{Tr}\left[\sigma_2 A\right]\,\right|^2}{4\|A\|^2}. \tag{2.15}$$

Here $\|A\|$ denotes the spectral norm of the matrix A, defined as

$$\|A\| \equiv \max_{\|x\|=1} \|Ax\|, \tag{2.16}$$

where the maximization is over vectors with (Euclidean) norm equal to 1 (even though we use the same notation for vector and spectral matrix norm, it should be clear from the context). For a Hermitian matrix the spectral norm is simply the largest of the modulus of the matrix's eigenvalues.

The weak-distinguishability, defined such that $0 \leq \widetilde{\mathcal{D}}_A \leq 1$, serves as a quantifier of distance: if $\widetilde{\mathcal{D}}_A\left(\sigma_1,\sigma_2\right) = 1$, then knowing the expectation value of A perfectly discriminates the two states, while if $\widetilde{\mathcal{D}}_A\left(\sigma_1,\sigma_2\right) = 0$ knowing the expectation value does not help us decide on whether the system is in state σ_1 or σ_2. Riemann used this same notion of distance to study the equilibration problem with respect to observables in [53].

Similarly to the previous section, we wish to upper-bound the time average of the weak-distinguishability between the instantaneous state ρ_t and the equilibrium state ω,

$$\left\langle \widetilde{\mathcal{D}}_A\left(\rho_t,\omega\right)\right\rangle_\infty = \lim_{T\to\infty}\frac{1}{T}\int_0^T \frac{\left|\mathrm{Tr}(\rho_t A) - \mathrm{Tr}(\omega A)\right|^2}{4\|A\|^2}dt. \tag{2.17}$$

We now follow the calculations by Short and Farrelly in [59]. By denoting the matrix elements of the observable in the energy basis as $A_{jk} \equiv \langle j| A |k\rangle$, and using the expression for the instantaneous state $\rho_t = \sum_{j,k}^{d_E} c_j c_k^* e^{-i(E_j - E_k)t} |j\rangle \langle k|$ and time averaged state $\omega = \sum_j^{d_E} |c_j|^2 |j\rangle \langle j|$, this expression can be rewritten as

$$\begin{aligned} \left\langle \widetilde{\mathcal{D}}_A(\rho_t, \omega) \right\rangle_\infty &= \left\langle \frac{|\mathrm{Tr}(\rho_t A) - \mathrm{Tr}(\omega A)|^2}{4\|A\|^2} \right\rangle_\infty \\ &= \frac{1}{4\|A\|^2} \left\langle \Big| \sum_{j,k}^{d_E} c_j c_k^* A_{kj} e^{-i(E_j - E_k)t} - \sum_j^{d_E} |c_j|^2 A_{jj} \Big|^2 \right\rangle_\infty \\ &= \frac{1}{4\|A\|^2} \sum_{j \neq k, l \neq m}^{d_E} (c_j c_k^* A_{kj})(c_l c_m^* A_{ml})^* \left\langle e^{-i[(E_j - E_k) - (E_l - E_m)]t} \right\rangle_\infty . \end{aligned} \tag{2.18}$$

We label each distinct pair of energy levels by indexes $\alpha = (j, k)$ and the corresponding energy gap by $G_\alpha \equiv E_j - E_k$. In this way a vector v and a Hermitian matrix M can be defined in the following manner:

$$v_\alpha \equiv c_j c_k^* \frac{A_{jk}}{\|A\|}, \qquad M_{\alpha\beta} \equiv \left\langle e^{-i(G_\alpha - G_\beta)t} \right\rangle_\infty . \tag{2.19}$$

The vector v contains information about the matrix elements of initial state and observable in the energy eigenbasis, while the matrix M involves the energy eigenvalues and time evolution. Notice that only terms with non-zero energy gaps appear in the sum since $\omega_{jk} = \rho_{jk}$ for $E_j = E_k$ [1].

With these definitions the time averaged weak-distinguishability has the very simple expression

$$\left\langle \widetilde{\mathcal{D}}_A(\rho_t, \omega) \right\rangle_\infty = \frac{1}{4} \sum_{\alpha\beta} v_\alpha M_{\alpha\beta} v_\beta^* . \tag{2.20}$$

We can now reproduce a result due to Reimann [53] (although we follow calculations by Short [56] and Short and Farrelly [59]).

Theorem 2.6 (Upper bound on the time averaged weak-distinguishability)**.** *For an observable A, Hamiltonian H with non-degenerate energy gaps, and an initial state ρ_0 with effective*

[1] Actually, in this case $\omega_{jk} = 0$ for $j \neq k$ since we are considering pure states, but in Chapter 4, when we perform a similar calculation, we will not impose such restriction.

dimension d_{eff},

$$\left\langle \widetilde{\mathcal{D}}_A\left(\rho_t,\omega\right)\right\rangle_\infty \leq \frac{1}{4d_{\text{eff}}}. \tag{2.21}$$

Proof. For any pair of different energy gaps, $M_{\alpha\beta} = \left\langle e^{-i(G_\alpha - G_\beta)t}\right\rangle_\infty = 0$. Therefore, the only terms in the sum that survive are the ones with $G_\alpha = G_\beta$, in which case $M_{\alpha\beta} = \delta_{\alpha\beta}$. Hence,

$$\begin{aligned}\left\langle \widetilde{\mathcal{D}}_A\left(\rho_t,\omega\right)\right\rangle_\infty &= \tfrac{1}{4}\sum_\alpha |v_\alpha|^2 \\ &= \tfrac{1}{4}\sum_{j\neq k} |c_j|^2|c_k|^2\frac{|A_{jk}|^2}{\|A\|^2} \\ &\leq \tfrac{1}{4}\sum_{j,k} |c_j|^2|c_k|^2\frac{|A_{jk}|^2}{\|A\|^2} \\ &= \tfrac{1}{4}\frac{\mathrm{Tr}(A\omega A\omega)}{\|A\|^2},\end{aligned} \tag{2.22}$$

Then, from using the fact that $(O,P) \equiv \mathrm{Tr}\left[O^\dagger P\right]$ defines an inner product (the Hilbert-Schmidt inner product [74]) and the Cauchy-Schwarz inequality in the first line, the fact that for any two positive semidefinite matrices $\mathrm{Tr}\left[OP\right] \leq \|O\|\,\mathrm{Tr}\left[P\right]$ in the second line, and that for pure states $\mathrm{Tr}\left[\omega^2\right] = \left(\sum_j^d |c_j|^2\right)^{-1} = 1/d_{\text{eff}}$ in the third line, we derive

$$\begin{aligned}\mathrm{Tr}(A\omega A\omega) &\leq \sqrt{\mathrm{Tr}(A^2\omega^2)\mathrm{Tr}(A^2\omega^2)} \\ &\leq \|A\|^2\mathrm{Tr}(\omega^2) \\ &= \frac{\|A\|^2}{d_{\text{eff}}}.\end{aligned} \tag{2.23}$$

Combining equations (2.22) and (2.23) finishes the proof.

□

Theorem 2.6 has a straightforward interpretation: as long as the effective dimension is large, the expectation value of *any* fixed observable equilibrates to its infinite time average.

However, simply comparing the expectation values of two distributions is not enough to differentiate between them. The weak-distinguishability actually defines a very weak

notion of distance. Nevertheless, as Short showed, the result for the weak-distinguishability can be used as a stepping stone to a much stricter result on equilibration, based on the *distinguishability*, defined as follows.

Definition 2.7 (Distinguishability)**.** *Given the measurement $\mathcal{M} = \{\mathcal{P}_1, \mathcal{P}_2, \ldots, \mathcal{P}_N\}$, where $\mathcal{P}_j$ are a complete set of projectors (or more generally, POVM's) corresponding to the different possible measurement outcomes, the distinguishability is defined by*

$$\mathcal{D}_{\mathcal{M}}(\sigma_1, \sigma_2) \equiv \frac{1}{2} \sum_{j}^{N} \left| \mathrm{Tr}\left[\sigma_1 \mathcal{P}_j\right] - \mathrm{Tr}\left[\sigma_2 \mathcal{P}_j\right] \right|. \tag{2.24}$$

The probability of successfully guessing between states σ_1 and σ_2 via the measurement $\mathcal{M}$ satisfies $p_{\text{success}} = \frac{1}{2}\left(1 + \mathcal{D}_{\mathcal{M}}(\sigma_1, \sigma_2)\right)$, assuming both states are given with equal probability. Hence we see that the distinguishability has a deeper physical significance than the weak-distinguishability. Moreover, it is worth noting that if one maximizes over all possible measurements the distinguishability equals the trace distance given by Defintion 2.2 is recovered [75].

Through the following lemma we can relate the distinguishability $\mathcal{D}_{\mathcal{M}}$ to the weak-distinguishability $\widetilde{\mathcal{D}}_{\mathcal{P}_j}$.

Lemma 2.8 (From weak-distinguishability to distinguishability)**.** *Given the measurement $\mathcal{M} = \{\mathcal{P}_1, \mathcal{P}_2, \ldots, \mathcal{P}_N\}$, where $\mathcal{P}_j$ are a complete set of projectors,*

$$\left\langle \mathcal{D}_{\mathcal{M}}(\rho_t, \omega) \right\rangle_T \leq \sqrt{N} \sqrt{\sum_{j}^{N} \left\langle \widetilde{\mathcal{D}}_{\mathcal{P}_j}(\rho_t, \omega) \right\rangle_T}. \tag{2.25}$$

Proof. Using Cauchy-Schwarz's inequality twice (in the first line for the space of continuous functions, and in the second line for vectors), we obtain

$$\begin{aligned}
\left\langle \mathcal{D}_{\mathcal{M}}(\rho_t, \omega) \right\rangle_T &\leq \sqrt{\left\langle \mathcal{D}^2_{\mathcal{M}}(\rho_t, \omega) \right\rangle_T} \\
&\leq \sqrt{N} \sqrt{\frac{1}{4} \sum_{i} \left\langle \left| \mathrm{Tr}\left[\mathcal{P}_j \rho_t\right] - \mathrm{Tr}\left[\mathcal{P}_j \omega\right] \right|^2 \right\rangle_T} \\
&= \sqrt{N} \sqrt{\sum_{j}^{N} \left\langle \widetilde{\mathcal{D}}_{\mathcal{P}_j}(\rho_t, \omega) \right\rangle_T}.
\end{aligned} \tag{2.26}$$

□

Each term $\left\langle \widetilde{\mathcal{D}}_{\mathcal{P}_j}(\rho_t, \omega) \right\rangle_T$ can now be bounded via Theorem 2.6 on page 18, which gives

$$\left\langle \mathcal{D}_{\mathcal{M}}(\rho_t, \omega) \right\rangle_T \leq \frac{N}{2\sqrt{d_{\text{eff}}}}. \tag{2.27}$$

Hence, as long as the number of measurement outputs considered is small compared to d_{eff} there is equilibration with respect to the distinguishability. Notice that in general the number of measurements one can reasonably take into account is much smaller than d_{eff}, since the latter typically grows exponentially with the constituents of the system being considered (see discussion on page 15).

Short also showed that equilibration with respect to observables can be used to recover the equilibration of a system in contact with an environment, reviewed in Section 2.1 on page 12. This justifies focusing solely on the observable equilibration viewpoint, which we will do from now on.

2.3 On the time scales of equilibration

2.3.1 Equilibration in a finite time

In the past two sections we saw that, under the non-degenerate gaps and high effective dimension assumptions, i) any fixed observable equilibrates, and ii) any system interacting with a large environment equilibrates. However, these results were obtained by performing an average over infinite time. In principle, these situations could correspond to systems which are out of equilibrium for extremely long times, as long as there is an even longer span of time in which the system is close to equilibrium (see Figure 2.3).

Knowing the *time scales* necessary to reach equilibrium is, in practice, as important as the results previously mentioned. For the case of a system interacting with an environment, the standard way in which this problem is usually addressed is via a master equation. These equations, derived by tracing out environmental degrees of freedom, approximate the evolution of a reduced density matrix by mimicking the effects of the environment [77]. However, unlike in the master equation approach, in this sections and the following chapters we prove

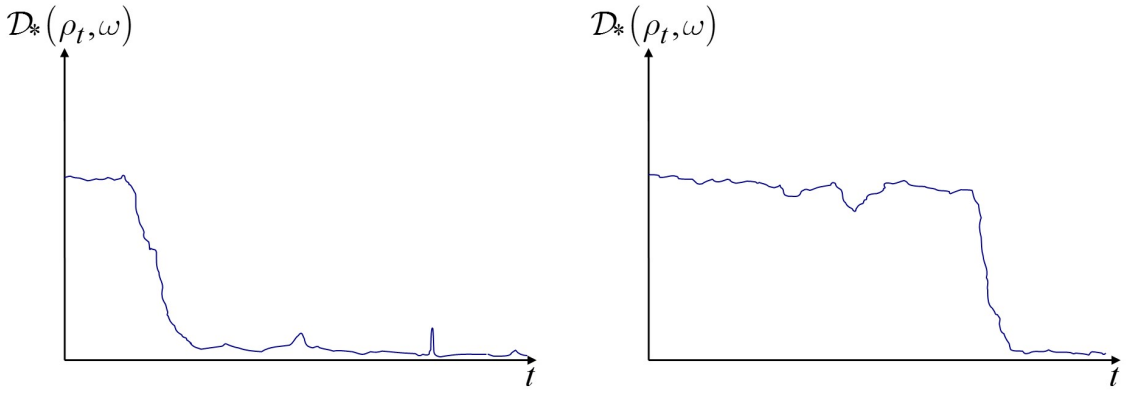

Figure 2.3: Illustration of short (left) and long (right) equilibration time scales.

everything from first principles without resorting to approximations. Moreover, while master equations specifically address the case of a small system interacting with an environment, the observable equilibration approach can be potentially extended to regimes not covered by master equations.

In order to focus on the time scale that the equilibration process takes, we extend Definition 2.1 on page 11 as follows.

Definition 2.9 (Finite time equilibration)**.** *A system equilibrates to the state ω with respect to the distance $\mathcal{D}_*$ and the equilibration constant χ in a finite time T if*

$$\left\langle \mathcal{D}_* \left(\rho_t, \omega\right) \right\rangle_T \leq \chi. \tag{2.28}$$

The smallest T such that the above holds will be referred to as the equilibration time scale T_{eq}, so that

$$\left\langle \mathcal{D}_* \left(\rho_t, \omega\right) \right\rangle_{T_{\text{eq}}} = \chi. \tag{2.29}$$

Proving that $\langle \mathcal{D}_* \left(\rho_t, \omega\right) \rangle_{T_{\text{eq}}}$ is small would imply that, for most times up to T_{eq}, the state ρ_t is close to the equilibrium state ω, with the meaning implied by the distance $\mathcal{D}_*$ chosen. In the same way as explained after eq. (2.5) on page 11, the fraction of times $t \in [0, T_{\text{eq}}]$ such that $\mathcal{D}_*(\rho_t, \omega) \geq \chi K$ would be smaller than $\frac{1}{K}$.

2.3.2 A general bound on the equilibration time scales

Short and Farrelly studied this problem, from a very general perspective, in [59]. We review their calculation, introducing a technical improvement that will result in a slightly tighter bound [68].

The main result of this section provides a general upper bound on the equilibration time scale.

Theorem 2.10. *For an observable A, Hamiltonian H and initial state ρ_0 with effective dimension d_{eff},*

$$\left\langle \widetilde{\mathcal{D}}_A\left(\rho_t - \omega\right)\right\rangle_T \leq \frac{5\pi}{8}\frac{\mathcal{N}(\epsilon)}{d_{\text{eff}}}\left(\frac{3}{2} + \frac{1}{\epsilon T}\right), \tag{2.30}$$

where $\mathcal{N}(\epsilon)$ is the maximum number of energy gaps that fit an energy interval of length ϵ,

$$\mathcal{N}(\epsilon) \equiv \max_E \left|\{\alpha : G_\alpha \in [E, E+\epsilon)\}\right|. \tag{2.31}$$

Proof. The mathematical trick to improve on Short and Farrelly's result comes from upper bounding the usual time average by a time average with a Lorentzian weight. If we define $\Theta_T(t) = \frac{1}{T}$ for $t \in [0, T]$ and 0 otherwise, the usual time average is $\langle f\rangle_T = \int_{-\infty}^{\infty} \Theta_T(t) f(t) dt$. Now notice that $\Theta_T(t) \leq \frac{5}{4}\frac{T}{T^2+(t-T/2)^2}$, hence for any positive function f one has $\langle f\left(t\right)\rangle_T \leq \frac{5\pi}{4}\langle f\left(t\right)\rangle_{L_T}$, with the Lorentzian time average (centered around $T/2$) denoted by

$$\langle f\rangle_{L_T} \equiv \int_{-\infty}^{\infty} \frac{1}{\pi}\frac{T}{T^2 + (t - T/2)^2} f(t) dt. \tag{2.32}$$

Since the weak-distinguishability is positive, we have

$$\left\langle \widetilde{\mathcal{D}}_A\left(\rho_t, \omega\right)\right\rangle_T \leq \frac{5\pi}{4}\left\langle \widetilde{\mathcal{D}}_A\left(\rho_t, \omega\right)\right\rangle_{L_T}. \tag{2.33}$$

Similarly as in the derivation of eq. (2.20) on page 18, we can write

$$\left\langle \widetilde{\mathcal{D}}_A\left(\rho_t, \omega\right)\right\rangle_{L_T} = \frac{1}{4}\sum_{\alpha\beta} v_\alpha M_{\alpha\beta}(T) v_\beta^*. \tag{2.34}$$

where the matrix $M(T)$ depends on the time averaging interval,

$$M_{\alpha\beta}(T) \equiv \left\langle e^{-i(G_\alpha - G_\beta)t} \right\rangle_{L_T}. \tag{2.35}$$

From this step we reproduce, for completeness, the calculations by Short and Farrelly. From the definition of the spectral norm $\|M(T)\|\|v\| \geq \|M(T)v\|$, so $\|v\|\|M(T)\|\|v\| \geq \|v\|\|M(T)v\| \geq |v^\dagger M(T)v|$. Hence,

$$\begin{aligned} \left\langle \widetilde{\mathcal{D}}_A\left(\rho_t, \omega\right) \right\rangle_T &= \tfrac{1}{4} \sum_{\alpha\beta} v_\alpha M_{\alpha\beta}(T) v_\beta^* \\ &\leq \tfrac{1}{4} \|M(T)\| \sum_\alpha |v_\alpha|^2. \end{aligned} \tag{2.36}$$

From the proof of Theorem 2.6 on page 18 we also know

$$\sum_\alpha |v_\alpha|^2 \leq \frac{1}{d_{\text{eff}}}. \tag{2.37}$$

Now we focus on upper bounding the norm of the matrix $M(T)$. By use of the identity $\langle e^{i\nu t} \rangle_{L_T} = e^{-|\nu|T} e^{i\nu T/2}$ (see the Fourier transform of a Lorentzian function, for example in [78]) we have $|M_{\alpha\beta}(T)| = \left| \left\langle e^{i(G_\alpha - G_\beta)t} \right\rangle_{L_T} \right| = e^{-|G_\alpha - G_\beta|T}$, and since $M(T)$ is a Hermitian matrix[2], its spectral norm satisfies

$$\|M(T)\| \leq \max_\beta \sum_\alpha |M_{\alpha\beta}(T)| = \max_\beta \sum_\alpha e^{-|G_\alpha - G_\beta|T}. \tag{2.38}$$

The sum can be divided into intervals of length ϵ, centered around a given gap G_β. An interval ϵ can fit at most $\mathcal{N}(\epsilon)$ gaps satisfying $(k + 1/2)\epsilon > G_\alpha - G_\beta > (k - 1/2)\epsilon$, which in turn implies that $|G_\alpha - G_\beta| \geq (|k| - 1/2)\epsilon$. Therefore

$$|M_{\alpha\beta}(T)| \leq e^{-(|k|-1/2)\epsilon T}. \tag{2.39}$$

For the case $k = 0$ we use the fact that $|M_{\alpha\beta}(T)| \leq 1$.

The sum is maximized by taking as many small values of $|k|$ as possible, and since there

[2]For any matrix M, its induced norms satisfy $\|M\| \equiv |||M|||_2 \leq \sqrt{|||M|||_1 |||M|||_\infty}$, where $|||M|||_1 \equiv \max_k \sum_j |M_{jk}|$ and $|||M|||_\infty \equiv \max_j \sum_k |M_{jk}|$ [73], and for Hermitian matrices $|||M|||_\infty = |||M|||_1$.

are $d_E(d_E-1)$ terms in total, we have that

$$\begin{aligned}\max_{\beta}\sum_{\alpha}|M_{\alpha\beta}(T)| &\leq \mathcal{N}(\epsilon)\left(1+2\sum_{k=1}^{d_E(d_E-1)}e^{-(k-1/2)\epsilon T}\right)\\ &= \mathcal{N}(\epsilon)\left(1+2e^{\epsilon T/2}\frac{e^{-\epsilon T}\left(e^{-\epsilon T d_E(d_E-1)}-1\right)}{e^{-\epsilon T}-1}\right)\\ &\leq \mathcal{N}(\epsilon)\left(1+2\frac{e^{-\epsilon T/2}}{1-e^{-\epsilon T}}\right).\end{aligned} \tag{2.40}$$

Finally, by using $\frac{1}{1-e^{-x}}\leq 1+\frac{1}{x}$, we obtain

$$\begin{aligned}\|M(T)\| &\leq \mathcal{N}(\epsilon)\left(1+2e^{-\epsilon T/2}+2\frac{e^{-\epsilon T/2}}{\epsilon T}\right)\\ &\leq \mathcal{N}(\epsilon)\left(3+\frac{2}{\epsilon T}\right).\end{aligned} \tag{2.41}$$

Combining this with equations (2.33), (2.36) and (2.37) completes the proof. □

In their original paper Short and Farrelly arrived at [3]

$$\left\langle \widetilde{\mathcal{D}}_A\left(\rho_t-\omega\right)\right\rangle_T \leq \frac{\mathcal{N}(\epsilon)}{4d_{\text{eff}}}\left(1+\frac{8\log_2(d_E)}{\epsilon T}\right), \tag{2.42}$$

which is worse by a factor scaling like $\sim\log_2(d_E)$. They also showed that this result can be used to obtain bounds on the time scale of equilibration with respect to the distinguishability, via similar calculations as in Lemma 2.8.

The strength of the result comes from its generality: the equilibration time scale T_{eq} that can be deduced from Theorem 2.10 holds for *any* observable.

A simple estimate serves to illustrate the magnitude of this bound. For simplicity, choose ϵ to be the minimum distance between gaps $\epsilon_{\min}$, and assume this minimum gap is non-degenerate, in which case $\mathcal{N}(\epsilon_{\min})=1$. If ΔE denotes the energy range where the state is supported, by noting that there are $d_E(d_E-1)$ energy gaps we see the minimum gap satisfies $\epsilon_{\min}\leq\frac{\Delta E}{d_E(d_E-1)}$, where the equality would correspond to the case when all the gaps are equally spaced. The energy standard deviation σ_E gives a fair estimate of the energy range,

[3] Bear in mind that we are focusing on the weak-distinguishability, which is up to a normalization constant the same as the quantity studied in [59].

and using that $d_E \geq d_{\text{eff}}$ results in an equilibration time that scales as

$$T_{\text{eq}} \sim \frac{1}{\chi} \frac{1}{d_{\text{eff}} \epsilon_{\text{min}}} \geq \frac{1}{\chi} \frac{d_{\text{eff}}}{\sigma_E} \sim \frac{1}{\chi} \frac{d_{\text{eff}}}{\sqrt{\log d_E}} \tag{2.43}$$

for an equilibration constant χ (see Definition 2.9 and Theorem 2.10), which is typically extremely long for systems composed of more than a few particles.

Herein resides the weakness of the result: it provides unsatisfactorily large bounds for any observable. In the next chapter we will investigate the reason why this general bound gives such long time scales, and search for observables for which equilibration happens in fast time scales. In turn, Chapter 4 will be about the quest for observables with physically physically realistic equilibration times.

Chapter 3

Extreme equilibration time scales

We devote this chapter to finding observables with extremely slow equilibration and observables with extremely rapid equilibration. In Section 3.1 we prove that for any pure system spread over many energy levels (i.e. with high effective dimension) it is always possible to define a measurement for which the equilibration time is tremendously long, essentially scaling with the dimension of the Hilbert space. On the other extreme, we find in Section 3.2 that, for any two-outcome measurement where one of the projectors is of small rank (logarithmically small in the dimension of the space), equilibration is extremely fast. We end in Secction 3.3 by showing that typical two-outcome measurements initially out of equilibrium also equilibrate very rapidly.

The previous chapter ended with a general bound on the equilibration time scales, valid for any observable A. We saw that estimates from this general bound gives extremely long time scales, which essentially grow with the dimension of the Hilbert space. A natural question that arises is whether a particular physical reason is behind these extremely long bounds, or, in other words, whether this upper bound is tight. On the other hand, our final goal is to find observables with more realistic evolutions, and in order to start probing this topic we will study the extreme of fast time scales. These two extremes will be the aim of this chapter, whose contents were a result of joint work with Artur S.L. Malabarba, Noah Linden, Terence C. Farrelly, and Anthony J. Short, and have been previously published as "Quantum Systems Equilibrate Rapidly for Most Observables", Phys. Rev. E **90**, 012121 (2014) [68].

In this chapter we restrict to simple measurements composed of two outcomes, $\mathcal{M} =$

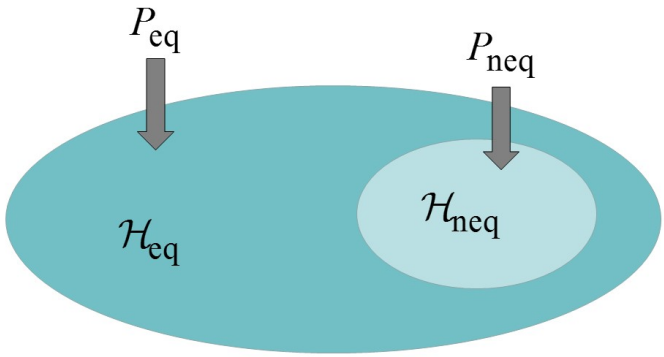

Figure 3.1: Consider an "equilibrium" space $\mathcal{H}_{\text{eq}}$ defined by states sharing some set of given properties, associated to equilibrium, and denote the orthogonal complement as $\mathcal{H}_{\text{neq}}$. In Goldstein et al. and Tasaki's viewpoint, any state with a high overlap with the orthogonal projector P_{eq} onto $\mathcal{H}_{\text{eq}}$ is said to be in equilibrium. In this setting the equilibration problem is related to understanding the conditions under which a state goes from the non-equilibrium to the equilibrium spaces, and can be mathematically stated in terms of the two-outcome measurement $\mathcal{M} = \{P_{\text{eq}}, P_{\text{neq}}\}$.

$\{P, \mathbb{1} - P\}$, and use the distinguishability to quantify distance between states. Such measurements find physical motivation in terms of *properties* assigned to systems. For instance, in the case of L spins, the projector $P = \sum_j^L |\uparrow\rangle \langle\uparrow|_j$, where $|\uparrow\rangle_j$ is the eigenvector of the Pauli z matrix, would be associated to the property "L spins point up in the z direction", and any state σ such that $\text{Tr}[\sigma P] \approx 1$ could be said to have such property. As a matter of fact, an approach to equilibration based on this notion has been advocated by Goldstein et al. [79] and Tasaki [80], which we briefly illustrate in Figure 3.1.

For two-outcome measurements the distinguishability becomes

$$\mathcal{D}_{\mathcal{M}}(\sigma_1, \sigma_2) \equiv \mathcal{D}_P(\sigma_1, \sigma_2) = \big|\, \text{Tr}[\sigma_1 P] - \text{Tr}[\sigma_2 P] \,\big|. \tag{3.1}$$

The energy standard deviation, defined as

$$\sigma_E \equiv \sqrt{\langle\psi| H^2 |\psi\rangle \; - \langle\psi| H |\psi\rangle^2}, \tag{3.2}$$

will serve as a reference scale for the times involved in the system's evolution, given that $\sim 1/\sigma_E$ characterizes a fast time scale in the system. To see this, consider the uncertainty relation between Hamiltonian H and an arbitrary observable A, which states $\sigma_E\sigma_A \geq \frac{1}{2}\big|\operatorname{Tr}\left[\rho_0[H,A]\right]\big| = \frac{1}{2}\left|\operatorname{Tr}\left[\rho_0\frac{dA}{dt}\right]\right|$ [81]. Thus, we see that the minimum necessary time for the expectation value of any observable to vary significantly with respect to its standard deviation σ_A satisfies $\frac{\sigma_A}{\left|\operatorname{Tr}\left[\rho_0\frac{dA}{dt}\right]\right|} \geq \frac{1}{2\sigma_E}$.

3.1 Slow Equilibration

In this section we show that for *any* pure system with high effective dimension, condition which ensures equilibration as we say in Chapter 2, it is always possible to define a measurement for which the equilibration time scale is extremely long. As a matter of fact, we find that these observables essentially saturate the general bound found by Short and Farrelly in [59], which we reviewed in Section section 2.3.2 on page 23.

Let us start by considering the projector $P_{\mathcal{H}_K}$ onto the subspace $\mathcal{H}_K$, which we define as

$$\mathcal{H}_K \equiv \operatorname{span}\left\{|\psi(j\tau)\rangle \;\middle|\; j = 0,\ldots,K-1\right\}, \tag{3.3}$$

where $\tau \equiv 2\epsilon/\sigma_E$ for some ϵ that will be chosen small, and $|\psi(t)\rangle$ is the (pure) state of the system at time t.

This construction is crucial for the following result.

Theorem 3.1 (Slow measurement)**.** *Given any Hamiltonian, any pure initial state $|\psi(0)\rangle$ with effective dimension d_{eff}, any positive integer $K \ll d_{\text{eff}}$ and $\epsilon > 0$, the distinguishability satisfies the following two equations*

$$\mathcal{D}_{P_{\mathcal{H}_K}}(\rho_t,\omega) \geq 1 - \epsilon^2 - \sqrt{\frac{K}{d_{\text{eff}}}}, \quad \forall t \in \left[0, K\tau - \frac{\epsilon}{\sigma_E}\right], \tag{3.4}$$

and

$$\left\langle \mathcal{D}_{P_{\mathcal{H}_K}}(\rho_t,\omega)\right\rangle_\infty \leq 2\sqrt{\frac{K}{d_{\text{eff}}}} \ll 1. \tag{3.5}$$

Proof. The constant ϵ is chosen small, so that $\tau = 2\epsilon/\sigma_E$ is a very small time step (as already mentioned, $1/\sigma_E$ is a characteristic fast time scale for the given system). Then the overlap

between the intial state $|\psi(0)\rangle$ and the state $|\psi(\tau)\rangle$ is nearly 1. To prove this we write $|\psi(t)\rangle$ in the energy basis

$$|\psi(t)\rangle = \sum_{j=1}^{d_E} c_j e^{-iE_j t} |j\rangle , \tag{3.6}$$

which allows seeing

$$\begin{aligned} \Big| \langle\psi(t)|\psi(0)\rangle \Big|^2 &= \left| \sum_{j=1}^{d_E} |c_j|^2 e^{-iE_j t} \right|^2 \\ &= \sum_{j,k=1}^{d_E} |c_j|^2 |c_k|^2 \cos\left((E_j - E_k)t\right) \\ &\geq 1 - \frac{t^2}{2} \sum_{j,k=1}^{d_E} |c_j|^2 |c_k|^2 \left(E_j^2 + E_k^2 - 2E_j E_k\right) \\ &= 1 - t^2 \sigma_E^2, \end{aligned} \tag{3.7}$$

by using that the energy standard deviation is $\sigma_E = \sqrt{\sum_j |c_j|^2 E_j^2 - \left(\sum_j |c_j|^2 E_j\right)^2}$. Hence, we have that

$$\Big| \langle\psi(t)|\psi(0)\rangle \Big|^2 \geq 1 - \epsilon^2, \tag{3.8}$$

for all t such that $|t| \leq \tau/2 = \epsilon/\sigma_E$. This trivially implies that $\forall\, t, t'$ such that $|t - t'| \leq \tau/2$,

$$\Big| \big\langle\psi(t)\big|\psi(t')\big\rangle \Big|^2 \geq 1 - \epsilon^2. \tag{3.9}$$

Meanwhile, by definition the subspace $\mathcal{H}_K$ contains all projectors $|\psi(j\tau)\rangle\langle\psi(j\tau)|$ for j up to $K-1$. Therefore, for any time t up to $(K - {}^1\!/_2)\tau$, the state $|\psi(t)\rangle$ is very close to one of these projectors.

In other words, there is always a value of $0 \leq j \leq K-1$ such that $|t - j\tau| \leq \tau/2$ and

$$\begin{aligned} \mathrm{Tr}\left[P_{\mathcal{H}_K} \rho_t\right] &= \langle\psi(t)| \left[P_{j\tau} + P_{j\tau}^{\perp}\right] |\psi(t)\rangle \\ &\geq \Big| \langle\psi(j\tau)|\psi(t)\rangle \Big|^2 \\ &\geq 1 - \epsilon^2, \end{aligned} \tag{3.10}$$

where $P_t \equiv |\psi(t)\rangle\langle\psi(t)|$ and $P_t^{\perp} \equiv P_{\mathcal{H}_K} - P_t$. From the Cauchy-Schwarz inequality we obtain $\mathrm{Tr}\left[P_{\mathcal{H}_K}\omega\right] \leq \sqrt{\mathrm{Tr}\left[P_{\mathcal{H}_K}^2\right]\mathrm{Tr}\left[\omega^2\right]} \leq \sqrt{\frac{K}{d_{\mathrm{eff}}}}$, since the subspace $\mathcal{H}_K$ contains all of the K projectors $|\psi(j\tau)\rangle\langle\psi(j\tau)|$. This leads to eq. (3.4):

$$\begin{aligned} D_{P_{\mathcal{H}_K}}(\rho_t, \omega) &= \left|\mathrm{Tr}\left[P_{\mathcal{H}_K}(\rho_t - \omega)\right]\right| \\ &\geq \mathrm{Tr}\left[P_{\mathcal{H}_K}\rho_t\right] - \mathrm{Tr}\left[P_{\mathcal{H}_K}\omega\right] \\ &\geq 1 - \epsilon^2 - \sqrt{\frac{K}{d_{\mathrm{eff}}}}. \end{aligned} \tag{3.11}$$

Eq. (3.5) is easily obtained from the Cauchy-Schwarz inequality

$$\begin{aligned} \left\langle D_{P_{\mathcal{H}_K}}(\rho_t, \omega)\right\rangle_{\infty} &= \left\langle\left|\mathrm{Tr}\left[P_{\mathcal{H}_K}(\rho_t - \omega)\right]\right|\right\rangle_{\infty} \\ &\leq \left\langle\mathrm{Tr}\left[P_{\mathcal{H}_K}\rho_t\right] + \mathrm{Tr}\left[P_{\mathcal{H}_K}\omega\right]\right\rangle_{\infty} \\ &= 2\,\mathrm{Tr}\left[P_{\mathcal{H}_K}\omega\right] \\ &\leq 2\sqrt{\mathrm{Tr}\left[{P_{\mathcal{H}_K}}^2\right]\mathrm{Tr}\left[\omega^2\right]} \\ &\leq 2\sqrt{\frac{K}{d_{\mathrm{eff}}}} \ll 1. \end{aligned} \tag{3.12}$$

□

Equation (3.4) on page 29 shows that, up to a time $K\tau - \epsilon/\sigma_E$, the system's state is distinguishable from its equilibrium state and has therefore not equilibrated, as long as ϵ and K are chosen appropriately so as to have $1 - \epsilon^2 - \sqrt{\frac{K}{d_{\mathrm{eff}}}}$ significantly above zero. On the other hand, eq. (3.5) shows that the system eventually equilibrates.

The proof essentially consists of constructing a subspace $\mathcal{H}_K$ which "traps" the state for a long period of time. This subspace is defined by K sequential "snapshots" of the system's state and, given a short enough time step τ between consecutive snapshots, makes sure that the system's state does not move out of $\mathcal{H}_K$ during the intermediate times. Even though one needs to take a small τ, the only requirement $K \ll d_{\mathrm{eff}}$ that is needed for equilibration to take place leaves a lot of room for K to be large, which results in a long total time $K\tau$.

For example, if we take $K = d_{\mathrm{eff}}/1000$ (typically an extremely large number) and $\epsilon = 1/2$,

we have from eq. (3.4) that

$$\mathcal{D}_{P_{\mathcal{H}_K}}(\rho_t, \omega) \geq \frac{1}{2}, \quad \forall t \in \left[0, \frac{d_{\text{eff}}}{1000\sigma_E}\right]. \tag{3.13}$$

For systems composed of a large number L of particles, one would usually expect the energy standard deviation to grow with the square root of the number of particles, $\sigma_E \sim \sqrt{L}$. Assuming the effective dimension grows linearly with the dimension of the Hilbert space d, and noticing that $d \sim e^{aL}$, leads to the system not having equilibrated with respect to this measurement up to a time which scales like $\sim \frac{d_{\text{eff}}}{\sqrt{\log(d_{\text{eff}})}}$. Notice that this is essentially the same scaling we found for the general bound on the equilibration time scale for any observable given by eq. (2.43) on page 26.

In order to illustrate how large such a time scale can be, let us consider a simple example. Take a system consisting of L weakly-interacting qubits with level-spacing $\delta E = 10^{-18}$Joules, the order of the excitation energy in atoms. Defining each qubit to have equal population on each level, simple calculations give $\sigma_E \approx \sqrt{L}\delta E$ and $d_{\text{eff}} \approx 2^L$, and we get $T_{\text{eq}}^{\text{slow}} > \frac{\hbar d_{\text{eff}}}{1000\sigma_E} \approx 2^L L^{-\frac{1}{2}} 10^{-19}\text{s}$ [1]. Then, taking as little as 125 qubits already gives $T_{\text{eq}}^{\text{slow}} \gtrsim 4.10^{17}$s, nearly the age of the universe, and increasing exponentially with L.

The construction given in Theorem 3.1 is not the only way that leads to observables with slow equilibration, and indeed an alternative one is given by Goldstein, Hara, and Tasaki in [63]. Their construction consists of considering a projector which only couples energy levels with energy gaps smaller than a certain value (that is, a projector whose matrix elements are non-zero only between energy levels of gaps smaller than a certain value). In this way, they ensure that only small frequencies are relevant in the evolution, which inevitably leads to a slow evolution.

These constructions leave an important lesson in the quest for understanding the equilibration time scales in closed quantum systems: even in a situation where general results exist that ensure that systems equilibrate with respect to any observable (i.e. states with high effective dimension, as we saw in Chapter 2), one can always find examples of observables for which the equilibration time scales are extremely long. On the one hand, this explains why the general approach taken by Short and Farrelly, which covered all observables, did not

[1] In this example we adopt S.I. units for illustration purposes.

provide a more reasonable result for the equilibration times. On the other hand, and this is the main message from this section, it means that restrictions are needed in order to identify the situations for which equilibration occurs in more physically realistic time scales.

3.2 Fast Equilibration

We now study the opposite extreme, in order to find sets of measurements for which equilibration is fast.

More precisely, we show that all systems with high effective dimension equilibrate fast with respect to the two-outcome measurement $\mathcal{M} = \{P, \mathbb{1} - P\}$, whenever the rank of either of the projectors is sufficiently small. Given $K \equiv \min\{\operatorname{rank} P, \operatorname{rank}(\mathbb{1} - P)\}$, we will prove that the average distinguishability $\langle \mathcal{D}_P(\rho_t, \omega)\rangle_T$ becomes small in a time scale of order K/σ_E.

Let us start by introducing the function $\xi_p(x)$, and a proposition related to it, which will be central to our following result [2].

Definition 3.2. *Given any normalized distribution p over the values of a real variable Y we define $\xi_p(x)$ as the maximum probability that fits an interval of length x. In particular, when Y is discrete,*

$$\xi_p(x) = \max_{y\in\mathbb{R}} \sum_{j:y_j\in[y,y+x]} p_j \tag{3.14}$$

For clarity, Figure 3.2 illustrates the function $\xi_p(x)$ for some arbitrary distribution p.

This function is central to the following proposition.

Proposition 3.3. *For a discrete distribution p_j on values y_j, and any $\gamma > 0$,*

$$\sum_{jk} p_j p_k e^{-\frac{|y_j - y_k|}{x}} \leq \frac{2}{1 - e^{-\gamma}} \xi_p(\gamma x). \tag{3.15}$$

Proof. Consider the auxiliary function

$$g(z) = \begin{cases} 1, \text{ if } z \in [0, 1) \\ 0, \text{ otherwise.} \end{cases} \tag{3.16}$$

[2] Notice we are using a different notation than in the original paper [68]

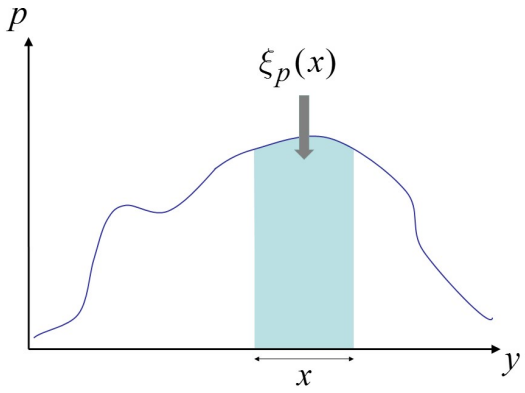

Figure 3.2: Graphic illustration of an arbitrary function $p(y)$, and the corresponding $\xi_p(x)$ quantifying the maximum probability inside an interval of length x, for some particular x.

The exponential function can be upper bounded as

$$e^{-|z|} \leq \sum_{n=0}^{\infty} e^{-\gamma n} g\left(\frac{|z|}{\gamma} - n\right). \tag{3.17}$$

By defining the intervals $I_+ = \big[y_+, y_+ + \gamma x\big)$ and $I_- = \big(y_- - \gamma x, y_-\big]$, where $y_\pm \equiv y_j \pm n\gamma x$, we see

$$\begin{aligned}
\sum_{jk} p_j p_k e^{-\frac{|y_j - y_k|}{x}} &\leq \sum_{n=0}^{\infty} e^{-\gamma n} \sum_j p_j \sum_k p_k g\left(\frac{|y_j - y_k|}{\gamma x} - n\right) \\
&= \sum_{n=0}^{\infty} e^{-\gamma n} \sum_j p_j \sum_{k\,:\left(\frac{|y_j - y_k|}{\gamma x} - n\right) \in [0,1)} p_k \\
&\leq \sum_{n=0}^{\infty} e^{-\gamma n} \sum_j p_j \left[\sum_{k\,:y_k \in I_-} p_k + \sum_{k\,:y_k \in I_+} p_k\right] \\
&\leq \sum_{n=0}^{\infty} e^{-\gamma n} \sum_j p_j \Big[2\xi_p\left(\gamma x\right)\Big] \\
&= \frac{2}{1 - e^{-\gamma}} \xi_p\left(\gamma x\right),
\end{aligned} \tag{3.18}$$

the inequality in the penultimate line being valid for any n and j. □

We now present the main result of this section, which gives an upper bound on the

finite-time average of the distinguishability $\mathcal{D}_P(\rho_t, \omega)$ for any projector P.

Theorem 3.4 (Fast equilibration)**.** *For any initial state ρ_0, any Hamiltonian, and any projector P with $K = \min\{\operatorname{rank} P, \operatorname{rank}(\mathbb{1} - P)\}$,*

$$\langle \mathcal{D}_P(\rho_t, \omega) \rangle_T \leq c\sqrt{\xi_\rho\left(\tfrac{1}{T}\right) K}, \tag{3.19}$$

where $c = \frac{5\pi}{4}\sqrt{\frac{2}{1-e^{-2}}} + 1 < 7$, and ξ_ρ given by Definition 3.2 on page 33, for the probability distribution defined by the diagonal elements of ρ in the energy eigenbasis, that is:

$$\xi_\rho(x) = \max_{E \in \mathbb{R}} \sum_{j : E_j \in [E, E+x]}^{d} \rho_{jj}. \tag{3.20}$$

Proof. As in the proof of Theorem 2.10 on page 23, we know that any positive function f satisfies $\langle f \rangle_T \leq \frac{5\pi}{4} \langle f \rangle_{L_T}$, where $\langle . \rangle_{L_T}$ denotes the Lorentzian time average. Then by use of the Cauchy-Schwarz inequality and the fact that $\operatorname{Tr}\left[\omega^2\right] \leq 1/d_{\text{eff}}$ [3],

$$\begin{aligned}
\langle \mathcal{D}_P(\rho_t, \omega) \rangle_T &= \left\langle \left| \operatorname{Tr}\left[P(\rho_t - \omega)\right] \right| \right\rangle_T \\
&\leq \langle \operatorname{Tr}\left[P\rho_t\right] \rangle_T + \operatorname{Tr}\left[P\omega\right] \\
&\leq \frac{5\pi}{4} \operatorname{Tr}\left[P\omega_{L_T}\right] + \sqrt{\operatorname{Tr}\left[\omega^2\right] \operatorname{Tr}\left[P^2\right]} \\
&\leq \frac{5\pi}{4} \sqrt{\operatorname{Tr}\left[\omega_{L_T}^2\right] \operatorname{Tr}\left[P^2\right]} + \sqrt{\operatorname{Tr}\left[\omega^2\right] \operatorname{Tr}\left[P^2\right]} \\
&\leq \frac{5\pi}{4} \sqrt{K \operatorname{Tr}\left[\omega_{L_T}^2\right]} + \sqrt{\frac{K}{d_{\text{eff}}}},
\end{aligned} \tag{3.21}$$

where $\omega_{L_T} \equiv \langle \rho_t \rangle_{L_T}$. The reason we may take $K = \min\{\operatorname{rank} P, \operatorname{rank}(\mathbb{1} - P)\}$ is that $D_P(\rho_t, \omega) = D_{\mathbb{1}-P}(\rho_t, \omega)\ \forall t \in \mathbb{R}$.

For a general initial state given by $\rho_0 = \sum_{jk} \rho_{jk} |j\rangle \langle k|$, we can write the purity of ω_{L_T}

[3] The equality holds for non-degenerate Hamiltonians or pure initial states, as in Definition 2.4 on page 14, while the inequality is necessary for degenerate Hamiltonians with a mixed initial state.

as

$$\begin{aligned}\mathrm{Tr}\left[\omega_{L_T}^2\right] &= \mathrm{Tr}\left[\sum_{j,k}\rho_{jk}\left\langle e^{-i(E_j-E_k)t}\right\rangle_{L_T}|j\rangle\ \langle k|\sum_{l,m}\rho_{lm}\left\langle e^{-i(E_l-E_m)t}\right\rangle_{L_T}|l\rangle\ \langle m|\right] \\ &= \sum_{j,k}|\rho_{jk}|^2\left|\left\langle e^{-i(E_j-E_k)t}\right\rangle_{L_T}\right|^2 \\ &\leq \sum_{j,k}\rho_{jj}\rho_{kk}\left|\left\langle e^{-i(E_j-E_k)t}\right\rangle_{L_T}\right|^2, \end{aligned} \tag{3.22}$$

where the last line is an equality for a pure initial state, and the inequality follows in general from positivity of the density operator [4].

By use of the identity $\left\langle e^{i\nu t}\right\rangle_{L_T} = e^{-|\nu|T}e^{i\nu T/2}$ we can in turn see

$$\mathrm{Tr}\left[\omega_{L_T}^2\right] \leq \sum_{jk}\rho_{jj}\rho_{kk}e^{-2|E_j-E_k|T}, \tag{3.23}$$

with the above being an equality for pure states.

Now we can apply Proposition 3.3 on page 33. For simplicity [5], we choose $\gamma = 2$, which results in

$$\mathrm{Tr}\left[\omega_{L_T}^2\right] \leq \frac{2}{1-e^{-2}}\xi_\rho\left(\frac{1}{T}\right), \tag{3.24}$$

and from eq. (3.21),

$$\langle\mathcal{D}_P(\rho_t,\omega)\rangle_T \leq \frac{5\pi}{4}\sqrt{\frac{2}{1-e^{-2}}}\sqrt{K\xi_\rho\left(\tfrac{1}{T}\right)} + \sqrt{\frac{K}{d_{\mathrm{eff}}}}. \tag{3.25}$$

Finally, using the fact that $d_{\mathrm{eff}}^{-1} \leq \max_j\{\rho_{jj}\} \leq \xi_\rho(x), \forall x > 0$ finishes the proof.

□

The purity of the time averaged state ω_{L_T} plays a predominant role in this result, dictating the evolution in the bound (3.21). The function $\xi_\rho\left(\frac{1}{T}\right)$ then serves as a route around having to calculate said purity, as eq. (3.24) shows. As we will see, estimating $\xi_\rho\left(\frac{1}{T}\right)$ turns out to be very simple. The general idea is that, for a rank-1 projector, for example, the measurement

[4] $\langle v|\,\rho\,|v\rangle \geq 0$ for all $|v\rangle$, which applies in particular to $|v\rangle = a\,|j\rangle + b\,|k\rangle$, so $\left(\begin{smallmatrix}\rho_{jj} & \rho_{jk}\\ \rho_{kj} & \rho_{kk}\end{smallmatrix}\right)$ is positive too, and, since the determinant must be greater than or equal to zero, $|\rho_{jk}|^2 \leq \rho_{jj}\rho_{kk}$.

[5] It would in principle be possible to keep the γ factor and optimize over its possible values at the end, but the improvement is minimal.

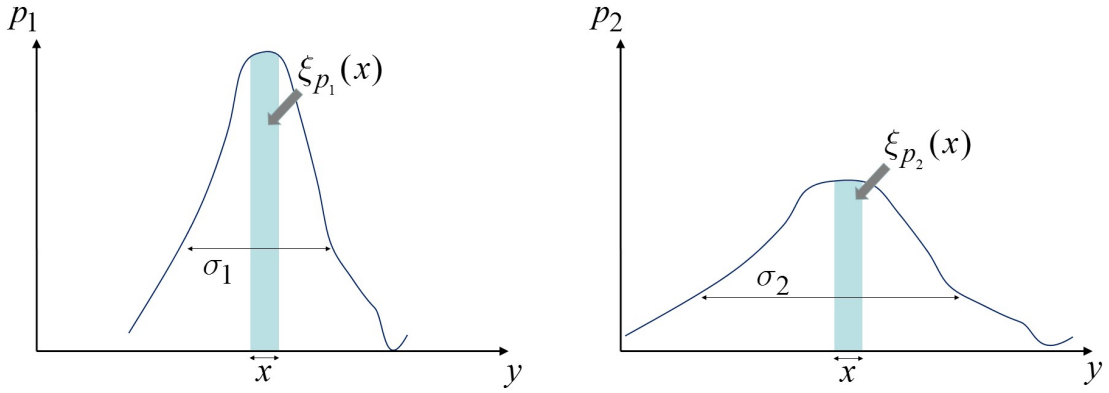

Figure 3.3: Illustration of the function $\xi_p(x)$ (light-blue area) for two arbitrary distributions p_1 and p_2, with standard deviations σ_1 and σ_2. For the distribution with higher dispersion less probability fits inside an interval of length x.

equilibrates as soon as the energy interval $\frac{1}{T}$ is too small to contain a significant portion of the probabilities. This roughly happens when $\frac{1}{T}$ is small compared to the energy standard deviation σ_E (see Figure 3.3 for an illustration of this), which as argued in the beginning of the chapter corresponds to a very short time scale. In turn, a rank-K projector would require that the probabilities be roughly K times smaller. Moreover, note that, as consequence of $d_{\text{eff}}^{-1} \leq \xi_\rho(x)$, a large d_{eff} is needed for equilibration to occur, as in the previous chapter, since $\xi_\rho\left(\frac{1}{T}\right)$ cannot converge to a small value otherwise.

3.2.1 Estimating ξ_ρ

In order to obtain a more concrete result for the time scale of equilibration, we can do a simple estimate of the behaviour of $\xi_\rho\left(\frac{1}{T}\right)$ as a function of time [6].

Given a dense enough energy spectrum, we can approximate the probability distribution of the initial state by a continuous function $\rho(E)$ for which the maximum value is roughly

$$\max_E \rho(E) \sim \frac{a}{\sigma_E}, \tag{3.26}$$

where a is some constant which depends on the shape of the distribution. Since $\xi_\rho(x)$ can

[6] The general arguments used here will be formalized in Section 4.2 on page 52.

always be upper bounded by $x \max_E \rho(E)$, we have

$$\xi_\rho\left(\frac{1}{T}\right) \lesssim \frac{a}{\sigma_E T}, \tag{3.27}$$

as long as T is not large enough such that the window of width $\frac{1}{T}$ only contains a few energy levels. In the next section we contrast this estimate with a concrete example, and obtain that, for example, for the case of a Gaussian distribution for the energy probabilities the above holds with $a \approx 0.40$.

This estimate then helps in determining the equilibration time scale. In accordance with Definition 2.9 on page 22, an upper bound for T_{eq} for this simple two-outcome measurement can be found from Theorem 3.4 via

$$\langle \mathcal{D}_P(\rho_t, \omega)\rangle_{T_{\text{eq}}} = \chi \leq c\sqrt{\xi_\rho\left(\tfrac{1}{T_{\text{eq}}}\right) K}, \tag{3.28}$$

for some reference equilibration constant χ. Using the estimate given by eq. (3.27) results in

$$T_{\text{eq}} \leq \frac{c^2 a}{\chi^2}\frac{K}{\sigma_E}. \tag{3.29}$$

This upper bound can be contrasted to the equilibration time scale of the slow observables found in Section 3.1. Considering the example on page 32, we obtain that for a rank-1 two outcome measurement, and for the same number of particles, the average distinguishability falls below $\chi = 10^{-3}$ in a time scale of $T_{\text{eq}}^{\text{fast}} \lesssim \frac{7000^2\hbar}{\sigma_E} \approx 4 \times 10^{-10}$s (assuming $a \sim 1$, taking $L = 125$, and $\sigma_E \sim \sqrt{L}\delta E$). This fast time scale, decreasing with $L^{-\frac{1}{2}}$, becomes unrealistically fast even for quite small systems.

Nevertheless, notice that most interesting measurements one can think of are actually of high rank. For instance, if as in the setting of Section 2.1 we consider a measurement on a small subsystem $\mathcal{S}$,

$$P = P_S \otimes \mathbb{1}_{\mathcal{E}}, \tag{3.30}$$

where P_S is a projector onto $\mathcal{S}$ and $\mathbb{1}_{\mathcal{E}}$ is the identity on the rest of the closed system (the environment), then $K = \text{rank}(P) \geq \text{rank}(\mathbb{1}_{\mathcal{E}}) = \frac{d}{d_S}$, extremely large even for modest sized environments. In such a case eq. (3.29) again results in an extremely long time scale,

essentially as long as the ones found in the previous section.

3.2.2 Gaussian Distribution Example

Let us now contrast our estimate for $\xi_\rho\left(\frac{1}{T}\right)$ with an example. Assume a pure initial state with a spectrum dense enough such that its probability distribution can be approximated by the following continuous function of energy

$$\rho(E) = \frac{1}{\sqrt{2\pi}\sigma_E} e^{-\frac{E^2}{2\sigma_E^2}}. \tag{3.31}$$

With this, we can bound the purity of ω_{L_T} via eq. (3.24) on page 36,

$$\mathrm{Tr}\left[\omega_{L_T}^2\right] \leq \frac{2}{1-e^{-2}}\xi_\rho\left(\frac{1}{T}\right) \leq 2.32\xi_\rho\left(\frac{1}{T}\right). \tag{3.32}$$

Since the density $\rho(E)$ is a Gaussian, $\xi_\rho\left(\frac{1}{T}\right)$ is obviously at its center. Thus, the estimate for ξ_ρ given by eq. 3.27 gives

$$\begin{aligned} \xi_\rho\left(\tfrac{1}{T}\right) &= \int_{-\frac{1}{2T}}^{\frac{1}{2T}} \frac{1}{\sqrt{2\pi}\sigma_E} e^{-\frac{E^2}{2\sigma_E^2}} dE \leq \frac{1}{\sqrt{2\pi}\sigma_E T}, \\ \mathrm{Tr}\left[\omega_{L_T}^2\right] &< \frac{3.28}{2\sqrt{\pi}\sigma_E T}, \end{aligned} \tag{3.33}$$

where the integral was trivially approximated by $\int_0^\epsilon \rho(E)dE < \epsilon\rho(0)$.

We now compare this result with the one obtained from using eq. (3.23) on page 36. The Fourier transform of the energy distribution is

$$\mu(t) = \int_{-\infty}^{\infty} \rho(E)e^{-iEt}dE = e^{-\frac{\sigma_E^2 t^2}{2}}. \tag{3.34}$$

Thus, using the continuous version of eq. (3.23), and taking into consideration that we

assumed a pure state,

$$\begin{aligned}
\mathrm{Tr}\left[\omega_{L_T}^2\right] &= \iint_{-\infty}^{\infty} dE\, dE'\, \rho(E)\rho(E') e^{-2|E-E'|T} \\
&= \iint_{-\infty}^{\infty} dE\, dE'\, \rho(E)\rho(E') \int_{-\infty}^{\infty} \frac{dt}{\pi} \frac{e^{i(E-E')2t} T}{T^2+t^2} \\
&= \int_{-\infty}^{\infty} \frac{dt}{\pi} \frac{T}{T^2+t^2} \left|\mu(2t)\right|^2 \\
&= \frac{T}{\pi} \int_{-\infty}^{\infty} \frac{e^{-4\sigma_E^2 t^2}}{T^2+t^2} dt \\
&= \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{e^{-4\sigma_E^2 T^2 x^2}}{1+x^2} dx \\
&= e^{4\sigma_E^2 T^2} \left(1 - \mathrm{erf}\left(2\sigma_E T\right)\right), \qquad (3.35)
\end{aligned}$$

where the second line uses the inverse Fourier transform of $e^{-2|E-E'|T}$. We can use the expansion of the Error Function

$$\mathrm{erf}(x) = 1 - \frac{e^{-x^2}}{\sqrt{\pi}x} + e^{-x^2}\mathcal{O}\left(x^{-3}\right) \qquad (3.36)$$

which, for $\sigma_E T$ large enough, results in

$$\mathrm{Tr}\left[\omega_{L_T}^2\right] \approx \frac{1}{2\sqrt{\pi}\sigma_E T}, \qquad (3.37)$$

for $\sigma_E T \gg 1$.

It is interesting to see that, despite the approximations taken, the function ξ_ρ gives good estimates for the purity of the average, with much simpler calculations.

Infinite Time Limit

The upper bounds we calculated in the example for $\mathrm{Tr}\left[\omega_{L_T}^2\right]$ tend to zero as T tends to infinity, which seems to contradict the fact that for the infinite time average state ω, $\mathrm{Tr}\left[\omega^2\right]$ is not zero. The reason this occurs is that one needs to be careful when averaging expressions like $\sum \rho_{jj}\rho_{kk} \exp[-2i(E_j - E_k)t]$ over energy levels. The terms with $E_j = E_k$ in the integrals arising from averages over $\rho(E)$ do not contribute (they are of measure zero), whereas in the finite sum they did, giving $\sum_{j=k} \rho_{jj}\rho_{kk} = 1/d_{\mathrm{eff}}$. Another way of looking at this is by noting

that taking the continuous limit implies taking $d_{\text{eff}} = \infty$.

3.3 Typical Measurements

In the previous two sections we studied the two extremes within the possible spectrum of time scales. Here we address the time scales of equilibration for typical measurements, suitably taken at random from the Haar measure, as we will see below. The statements will involve typical two-outcome measurements composed of a projector of *any* rank, applied to any initial state and any Hamiltonian. The lengthier calculations can be found in Appendix A.1 on page 95.

The following lemma will be central to our results (see for example [82], or Section 3.2 of [83]).

Lemma 3.5. *For any operator M,*

$$\left\langle U^{\otimes 2} M (U^{\otimes 2})^\dagger \right\rangle_U = \alpha \Pi_S + \beta \Pi_A, \tag{3.38}$$

where $\Pi_S \equiv (\mathbb{1}^{\otimes 2} + \$)/2$ and $\Pi_A \equiv (\mathbb{1}^{\otimes 2} - \$)/2$ are projectors with ranks $\frac{d(d+1)}{2}$ and $\frac{d(d-1)}{2}$ respectively, and $\$ is the swap operator on $\mathcal{H} \otimes \mathcal{H}$, defined by: $\$ \left|a\right\rangle \left|b\right\rangle = \left|b\right\rangle \left|a\right\rangle$.

This lemma will be particularly useful to us for the case $M = P^{\otimes 2}$, where we get

$$\begin{aligned} \alpha &= \frac{\operatorname{Tr}\left[\Pi_S P^{\otimes 2}\right]}{\operatorname{Tr}\left[\Pi_S\right]} = \frac{1}{d(d+1)} \left[\operatorname{Tr}\left[P \otimes P\right] + \operatorname{Tr}\left[P^2\right]\right] \\ &= \frac{K(K+1)}{d(d+1)}, \end{aligned} \tag{3.39}$$

by using that $\operatorname{Tr}\left[\$ \, A \otimes B\right] = \operatorname{Tr}\left[AB\right]$. A similar calculation gives

$$\begin{aligned} \beta &= \frac{\operatorname{Tr}\left[\Pi_A P_U^{\otimes 2}\right]}{\operatorname{Tr}\left[\Pi_A\right]} \\ &= \frac{K(K-1)}{d(d-1)}. \end{aligned} \tag{3.40}$$

This allows proving the following simple result, which points to the fact that not any typical measurement is of interest for the equilibration process.

Theorem 3.6 (Typical two-outcome measurements are already equilibrated)**.** *Consider the rank-K projector P_U defined as the unitary transformation from an energy basis projector*

$$P_U = UPU^\dagger = \sum_{j=1}^{K} U\left|j\right\rangle \left\langle j\right| U^\dagger, \tag{3.41}$$

with $U : \mathcal{H} \to \mathcal{H}$ unitary and $|j\rangle$ being eigenstates of the Hamiltonian H.

Then, for any initial state ρ, the distinguishability between $\rho_t = e^{-iHt}\rho_0 e^{iHt}$ and ω according to P_U (and its complement) averaged over all unitaries satisfies

$$\left\langle \mathcal{D}_{P_U}(\rho_t, \omega)\right\rangle_U \leq \sqrt{\frac{K}{d^2}\frac{d-K}{d+1}} \leq \frac{1}{2\sqrt{d+1}}. \tag{3.42}$$

Proof. From Jensen's inequality we get [84]

$$\left\langle \mathcal{D}_{P_U}(\rho_t, \omega)\right\rangle_U \leq \sqrt{\left\langle \mathcal{D}_{P_U}(\rho_t, \omega)^2\right\rangle_U}. \tag{3.43}$$

Now the average of the squared distinguishability can be exactly calculated to be

$$\begin{aligned}
\left\langle \mathcal{D}_{P_U}(\rho_t, \omega)^2\right\rangle_U &= \left\langle \left(\operatorname{Tr}\left[P_U(\rho_t - \omega)\right]\right)^2\right\rangle_U \\
&= \operatorname{Tr}\left[\left\langle P_U \otimes P_U\right\rangle_U (\rho_t - \omega)^{\otimes 2}\right]. \\
&= \operatorname{Tr}\left[\left(\alpha\Pi_S + \beta\Pi_A\right)(\rho_t - \omega) \otimes (\rho_t - \omega)\right] \\
&= \frac{\alpha+\beta}{2}\left(\operatorname{Tr}\left[\rho_t - \omega\right]\right)^2 + \frac{\alpha-\beta}{2}\operatorname{Tr}\left[(\rho_t - \omega)^2\right] \\
&= \frac{K}{2d}\left(\frac{K+1}{d+1} - \frac{K-1}{d-1}\right)\left(\operatorname{Tr}\left[\rho_t^2\right] + \operatorname{Tr}\left[\omega^2\right] - 2\operatorname{Tr}\left[\rho_t\omega\right]\right) \\
&= \frac{K}{d}\frac{d-K}{d^2-1}\operatorname{Tr}\left[\rho_t^2 - \omega^2\right],
\end{aligned} \tag{3.44}$$

by using eqs. (3.39) and (3.40), plus the fact that $\operatorname{Tr}\left[\rho_t\omega\right] = \operatorname{Tr}\left[\omega^2\right]$.

Since the purity of the state is minimized for $\omega = \mathbb{1}/d$ we have $\operatorname{Tr}\left[\omega^2\right] \geq 1/d$, which implies that $\operatorname{Tr}\left[\rho_t^2 - \omega^2\right] \leq (d-1)/d$, and leads to the first inequality of eq. (3.42). The second inequality is obtained by setting $K = d/2$, which maximizes the expression. □

This theorem shows that for most times the distinguishability of a typical measurement

is small for systems with a high dimension d. However, it does not make any statements about time scales or the dynamics of the equilibration process. For this purpose, it is more relevant to study measurements which start out of equilibrium in the first place, and ask how fast they approach it.

Therefore, we now constrain the projector to start out of equilibrium. This is ensured by imposing that $\rho_0 = |\Psi\rangle\langle\Psi|$ is one of the projector's terms (note that for this theorem, we restrict the initial state to be pure). In order to achieve this, the Hilbert space is divided between the span of the initial state and everything else, $\mathcal{H} = \mathcal{H}' \oplus \rho_0$, where $\dim \mathcal{H} = d$ and $\dim \mathcal{H}' = d - 1$. These observables are typically out of equilibrium initially, as the following lemma shows.

Lemma 3.7 (Observables with a definite initial value are typically out of equilibrium)**.** *Consider the projector given by*

$$\Pi_U = \rho_0 + P_U, \qquad P_U = UPU^\dagger, \tag{3.45}$$

where ρ_0 is the initial (pure) state, U is a partial unitary with $UU^\dagger = U^\dagger U = \mathbb{1}_{\mathcal{H}'}$, P is any rank-$(K-1)$ projector with support on $\mathcal{H}'$. Then, the distinguishability between ρ_0 and ω according to Π_U (and its complement) averaged over all unitaries on $\mathcal{H}'$ satisfies

$$\langle \mathcal{D}_{\Pi_U}(\rho_0, \omega)\rangle_U \geq \left(1 - \frac{K-1}{d-1}\right)\left(1 - \frac{1}{d_{\text{eff}}}\right). \tag{3.46}$$

Proof. To simplify notation in the following proofs, we assume $d > 2$, and set $d' \equiv \dim \mathcal{H}' = d - 1$ and $K' \equiv \operatorname{rank} P_U = K - 1$. To show that observables with a definite initial value are typically out of equilibrium, we consider the initial distinguishability between ρ_0 and ω for

a measurement of Π_U, averaged over U:

$$\begin{aligned}
\langle \mathcal{D}_{\Pi_U}(\rho_0, \omega)\rangle_U &= \langle |\mathrm{Tr}\left[\Pi_U(\rho_0 - \omega)\right]|\rangle_U \\
&= \langle (1 - \mathrm{Tr}\left[\Pi_U \omega\right])\rangle_U \\
&= 1 - \mathrm{Tr}\left[\left[\rho_0 + \frac{K'}{d'}(\mathbb{1} - \rho_0)\right]\omega\right] \\
&= \left(1 - \frac{K'}{d'}\right)(1 - \mathrm{Tr}\left[\rho_0 \omega\right]) \\
&\geq \left(1 - \frac{K-1}{d-1}\right)\left(1 - \frac{1}{d_{\mathrm{eff}}}\right),
\end{aligned} \tag{3.47}$$

where the third line comes from the fact that $\langle UPU^\dagger\rangle_U \propto \mathbb{1}_{\mathcal{H}'}$, and the last line is an equality if ρ_0 is pure.

□

This lemma shows that the typical distinguishability for these measurements is significantly above zero as long as the projector does not cover almost the entire space (that is, as long as $K \ll d$), and therefore start out of equilibrium

Nevertheless, there is a non-trivial equilibration process, which we prove as follows.

Theorem 3.8 (Typical two-outcome measurements with a definite initial value equilibrate fast for any pure initial state with high d_{eff})**.** *Consider the projector given by*

$$\Pi_U = \rho_0 + P_U, \qquad P_U = UPU^\dagger, \tag{3.48}$$

where ρ_0 is the initial (pure) state, U is a partial unitary with $UU^\dagger = U^\dagger U = \mathbb{1}_{\mathcal{H}'}$, P is any rank-$(K-1)$ projector with support on $\mathcal{H}'$.

The distinguishability between ρ_t and ω according to Π_U (and its complement) averaged over all unitaries on $\mathcal{H}'$ satisfies

$$\langle \mathcal{D}_{\Pi_U}(\rho_t, \omega)\rangle_U \leq \mathcal{D}_{\rho_0}(\rho_t, \omega) + \frac{1}{2\sqrt{d-1}}, \tag{3.49}$$

which together with Theorems 3.4 and 3.6 on pages 35 and 42 imply that

$$\left\langle \langle \mathcal{D}_{\Pi_U}(\rho_t, \omega)\rangle_U \right\rangle_T \leq c\sqrt{\xi_\rho\left(\tfrac{1}{T}\right)} + \frac{1}{2\sqrt{d-1}} \tag{3.50}$$

decays very fast, with $c < 7$.

The proof is found in Appendix A.1.1 on page 95. This result shows that most two-outcome measurements (of any rank) containing the initial state equilibrate as fast as the measurement of the rank-1 projector consisting of *only* the initial state.

Moreover, we can extend the previous results to multi-outcome measurements.

Corollary 3.9 (N-outcome generalization of Theorem 3.6)**.** *Given* $N \ll d$*, the typical* N*-outcome measurement is already equilibrated. Describing the measurement by the POVM* $\mathcal{M}_U = \left\{U^\dagger P_i U\right\}_{i=1,N}$*, and using the result from Theorem 3.6, it is easy to see that*

$$\begin{aligned}\langle \mathcal{D}_{\mathcal{M}_U}(\rho_t, \omega)\rangle_U &= \frac{1}{2}\sum_{j=1}^{N}\left\langle \mathcal{D}_{U^\dagger P_j U}(\rho_t, \omega)\right\rangle_U \\ &\leq \frac{1}{2}\sum_{j=1}^{N}\sqrt{\frac{K_j}{d^2}\frac{d-K_j}{d+1}} \\ &\leq \frac{1}{2}\sqrt{\frac{N}{d+1}}\end{aligned} \tag{3.51}$$

where $K_j = \operatorname{rank} P_j$*, and the second line is maximal for* $K_j = d/N$.

Corollary 3.10 (N-outcome generalization of Theorem 3.8)**.** *Given* $N \ll d$*, typical out-of-equilibrium* N*-outcome measurements equilibrate fast for any pure initial state with high* d_{eff}*. Consider the POVM given by the measurements* $\mathcal{M}_U^{\rho_0} = \left\{\rho_0 + U^\dagger P_1 U,\ U^\dagger P_2 U,\ \ldots,\ U^\dagger P_N U\right\}$*, with* $\rho_0 + \sum U^\dagger P_n U = \mathbb{1}$*. We show in Appendix A.1.2, that*

$$\left\langle \mathcal{D}_{\mathcal{M}_U^{\rho_0}}(\rho_t, \omega)\right\rangle_U \leq \mathcal{D}_{\rho_0}(\rho_t, \omega) + \frac{1}{2}\sqrt{\frac{N}{d-1}}. \tag{3.52}$$

This means that most measurements are already equilibrated even for a large number of outcomes as long as $N \ll d$, a physically reasonable assumption for systems composed of many particles given that the dimension d grows exponentially with the number particles.

Furthermore, for any $N \ll d$, most measurements with a definite initial value (which are typically out of equilibrium initially) still equilibrate essentially as fast as a rank-1 projector.

We thus see that these typical measurements starting out of equilibrium equilibrate as fast as rank-1 measurements, which, as we saw in Section 3.2.1, essentially equilibrate on a time scale $\sim 1/\sigma_E$. As eq. (3.29) on page 38 illustrates, this is an extremely fast time scale; an unrealistically fast one in fact compared to what typically occurs in nature.

Firstly, this reinforces our previous statement regarding the need to impose further conditions on the measurements being considered in order to prove physically realistic equilibration time scales.

On the other hand, the unrealistically fast time scales obtained from Theorem 3.8 can also be seen as manifesting the fact that typical in the Haar measure sense need not reflect typical in the physical sense, particularly with regards to the equilibration problem. This shortcoming was already made clear in an article by Cramer [85]. The author builds up on the previous work of Vinayak and Žnidarič [60], Brandão et al. [61], and Masanes, Roncaglia and Acín [62], studying the equilibration time scales of small subsystems under a random system-environment Hamiltonian with a fixed spectrum. In the paper, Cramer proves that in such instances the equilibrium state of the subsystem is $\omega_S = \frac{\mathbb{1}_S}{d_S}$, which corresponds to an equilibration to an infinite temperature state, clearly not physically typical. It is also worth noting that the time scales found by Vinayak and Žnidarič, Brandão et al., and Masanes, Roncaglia and Acín, essentially coincide with the ones found in this section for typical measurements.

In summary, we have found measurements with extremely slow and measurements with extremely fast equilibration. For any system in a pure initial state with high effective dimension, the measurements constructed in Section 3.1 had times scaling like

$$T_{\text{eq}}^{\text{slow}} \gtrsim \frac{d_{\text{eff}}}{\sigma_E}, \tag{3.53}$$

while for small rank two-outcome measurements and any any initial state we found in Section 3.2 times scaling like

$$T_{\text{eq}}^{\text{fast}} \lesssim \frac{K}{\sigma_E}, \tag{3.54}$$

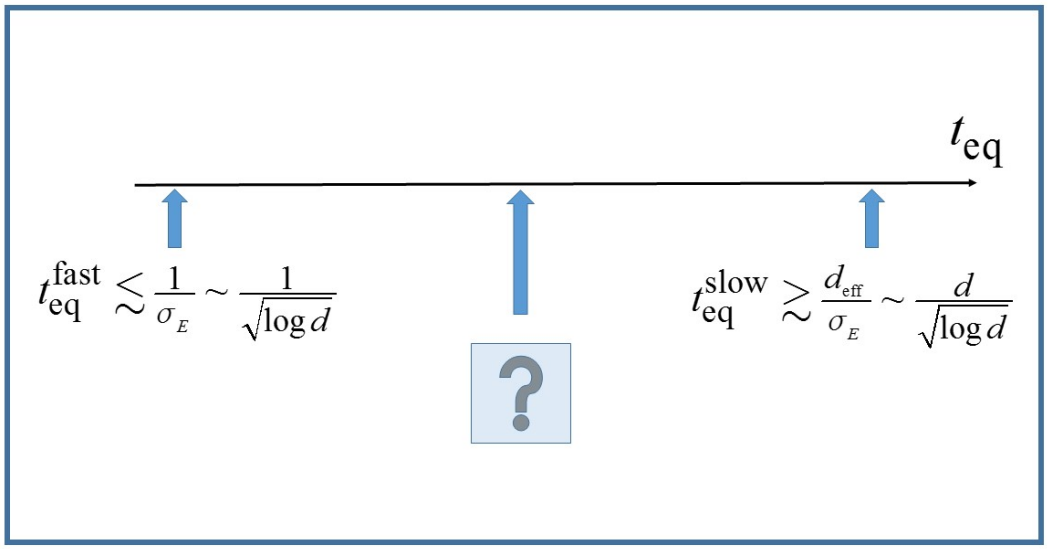

Figure 3.4: Illustration of how the equilibration times found in this chapter scale. Even for relatively small systems $T_{\text{eq}}^{\text{fast}}$ becomes too small while $T_{\text{eq}}^{\text{slow}}$ becomes too large, given the rapid increase of the dimension of the Hilbert space with the size of the system. For physically relevant measurements, like a measurement on a small subsystem, the fast timescale $T_{\text{eq}}^{\text{fast}} \lesssim \frac{K}{\sigma_E}$ falls to the slow extreme, since $K \sim d$. The middle of the spectrum remains an open question, that we will address in the next chapter

which for $K = 1$ also characterizes the time scale for the typical measurements considered in this section. As mentioned, most physical observables one can think of actually have very large ranks, in which case the above time scale becomes extremely large.

Both of the time scale extremes found in this chapter, which we illustrate in Figure 3.4, are unrealistic. Finding observables which fall withing the middle of the spectrum for physically realistic setups will be the aim of next chapter.

Chapter 4

The quest for physically realistic time scales

The aim of this chapter is to find conditions under which equilibration can be proven to occur in more realistic time scales than for the observables found in Chapter 3. We start in Section 4.1 by proving a new general upper bound on the time averaged distance between instantaneous and equilibrium state. Section 4.2 is devoted to the time decay of the previously mentioned general result, while Section 4.3 contains an expression for the time scale of equilibration which depends on the observable, state and Hamiltonian under consideration; the first main result of the chapter. In 4.4 we apply the result to the case of a system interacting with a thermal bath in the microcanonical ensemble, an important application of the previous part. We end in Section 4.5 with a discussion of the conditions necessary to obtain realistic equilibration times.

The quest for proving realistic time scales of equilibration necessarily involves restrictions. Otherwise, one could end up with the observables with extremely slow equilibration found in Chapter 3. These restrictions must necessarily involve the relevant physical quantities for the dynamics, namely the Hamiltonian, the initial state, and the observable. This chapter, devoted to our effort in finding a set of conditions on this dynamic trio $\{H, \rho_0, A\}$ under which physically realistic time scales can be proven, is a result of joint work with Noah Linden, Artur S.L. Malabarba, Anthony J. Short and Andreas Winter, and can be found as the preprint "Equilibration time scales of physically relevant observables", arXiv:1509.05732 [69].

4.1 Bound on average distance

As before, let us consider a closed quantum system with a Hamiltonian H, and an initial state given by the density matrix ρ_0 in a Hilbert space $\mathcal{H}$. Along this chapter, given an Hermitian operator A, we will adopt the weak-distinguishability $\widetilde{\mathcal{D}}_A(\sigma_1,\sigma_2) \equiv \frac{1}{4\|A\|^2}\big|\operatorname{Tr}[\sigma_1 A] - \operatorname{Tr}[\sigma_2 A]\big|^2$ as a notion of distance between any two states σ_1 and σ_2 (see Definition 2.5 on page 17). Nevertheless, the calculations based on this weak notion of distance could be extended to a stricter notion of equilibration, the distinguishability, by Lemma 2.8 on page 20.

The same way as we did in Section 2.2 (see page 18), the time average of the weak-distinguishability between instantaneous state ρ_t and equilibrium state ω can be written as

$$\begin{aligned}\Big\langle \widetilde{\mathcal{D}}_A(\rho_t,\omega)\Big\rangle_T &= \frac{1}{4}\left\langle \Big| \sum_{j,k} e^{-i(E_j-E_k)t}(\rho_{jk}-\omega_{jk})\frac{A_{kj}}{\|A\|}\Big|^2 \right\rangle_T \\ &= \frac{1}{4}\left\langle \Big| \sum_{\alpha} v_\alpha e^{-iG_\alpha t}\Big|^2 \right\rangle_T \\ &= \frac{1}{4}\sum_{\alpha\beta} v_\alpha v_\beta^* \left\langle e^{-i(G_\alpha - G_\beta)t}\right\rangle_T, \end{aligned} \tag{4.1}$$

where the the energy gaps $G_\alpha = (E_j - E_k)$ are identified with Greek indexes α representing pairs (j,k) of levels with distinct energies, and the coefficients

$$v_\alpha \equiv v_{(j,k)} = \rho_{jk}\frac{A_{kj}}{\|A\|} \tag{4.2}$$

encompass all matrix elements of observable and initial state in the energy basis.

Once again, we aim to prove that the time average of the weak-distinguishability considered above becomes small, which would allow us to conclude that for most times the weak-distinguishability is small, showing equilibration occurs. Firstly, we obtain the following.

Proposition 4.1 (General bound)**.** *For any initial state ρ_0, any Hamiltonian, and any observable A,*

$$\Big\langle \widetilde{\mathcal{D}}_A(\rho_t,\omega)\Big\rangle_T \leq cQ^2\xi_p\big(\tfrac{1}{T}\big), \tag{4.3}$$

where $c \equiv \frac{\pi}{1-e^{-1}} < 5$*, and for the normalized distribution* p_α

$$p_\alpha \equiv \frac{|v_\alpha|}{Q}, \qquad Q \equiv \sum_\alpha |v_\alpha|, \tag{4.4}$$

the function

$$\xi_p(x) \equiv \max_G \sum_{\alpha: G_\alpha \in [G, G+x]} p_\alpha, \tag{4.5}$$

given by Definition 3.2 on page 33, quantifies the maximum probability that fits an energy interval of length x*.*

Proof. We start by noting that, since $\widetilde{\mathcal{D}}_A$ is a positive quantity,

$$\left\langle \widetilde{\mathcal{D}}_A(\rho_t, \omega) \right\rangle_T \leq 2\pi \left\langle \widetilde{\mathcal{D}}_A(\rho_t, \omega) \right\rangle_{L_T}, \tag{4.6}$$

where $\langle f(t) \rangle_{L_T} \equiv \int_{-\infty}^{\infty} \frac{f(t)T}{T^2+t^2} \frac{dt}{\pi}$ denotes the Lorentzian time average of the function f. As we did in Section 2.3.2, the above is easily shown by defining $\Theta_T(t) = \frac{1}{T}$ for $t \in [0, T]$ and 0 otherwise. Then $\langle f \rangle_T = \int_{-\infty}^{\infty} \Theta_T(t) f(t) dt$, and using $\Theta_T(t) \leq 2\frac{T}{T^2+t^2}$ proves the bound. Notice that in this case it will prove useful to take the Lorentzian average centered around 0, unlike in Section 2.3.2 where the average was centered around $\frac{T}{2}$.

Upper bounding the sum in eq. (4.1) by taking the absolute values of each term, incorporating eq. (4.6), and using that $\langle e^{i\nu t} \rangle_{L_T} = e^{-|\nu|T}$, we get

$$\left\langle \widetilde{\mathcal{D}}_A(\rho_t, \omega) \right\rangle_T \leq \frac{\pi Q^2}{2} \sum_{\alpha\beta} p_\alpha p_\beta e^{-|G_\alpha - G_\beta|T}. \tag{4.7}$$

In order to finish the proof we apply Proposition 3.3 on page 33, with $\gamma = 1$.

□

In the next section we consider general properties of $\xi_p(x)$ that will prove useful in studying the decay in time of the time averaged weak-distinguishability.

4.2 Bounding $\xi_p(x)$

The function $\xi_p(x)$ will in general be difficult to compute explicitly, but for small x it can be bounded (and well approximated) by a linear function. We will capture this behaviour in the following.

Proposition 4.2. *For any distribution p,*

$$\xi_p(x) \leq \frac{\xi_p(\epsilon)}{\epsilon} x + \xi_p(\epsilon), \qquad \forall \epsilon \in (0, \infty). \tag{4.8}$$

It will be convenient to re-express this as

$$\xi_p(x) \leq \frac{a(\epsilon)}{\sigma} x + \delta(\epsilon), \tag{4.9}$$

where σ is the standard deviation of the distribution, and we define

$$a(\epsilon) = \frac{\xi_p(\epsilon)}{\epsilon}\sigma, \qquad \delta(\epsilon) = \xi_p(\epsilon). \tag{4.10}$$

Proof. Take $(n-1)\,\epsilon \leq x < n\epsilon$, with $n \geq 1$ a natural number. The function ξ_p is non-decreasing, hence $\xi_p(x) \leq \xi_p(n\epsilon)$. Since $\xi_p(\epsilon)$ quantifies the maximum probability that can fit *any* interval ϵ, we also have that $\xi_p(n\epsilon) \leq n\xi_p(\epsilon)$, which results in

$$\begin{aligned} \xi_p(x) &\leq \xi_p(n\epsilon) \leq (n-1)\xi_p(\epsilon) + \xi_p(\epsilon) \\ &\leq \frac{\xi_p(\epsilon)}{\epsilon} x + \xi_p(\epsilon). \end{aligned} \tag{4.11}$$

□

We now derive some general properties of ξ_p. For many distributions p we would expect to be able to find an ϵ such that $a(\epsilon) \sim 1$ (in terms of its approximate order of magnitude) and $\delta(\epsilon) \ll 1$. To visualize how this can be so, consider the case in which the distribution has essentially a single "peak", and that the standard deviation σ approximately quantifies the width of this peak. In such a case, a rough estimate for the maximum probability that

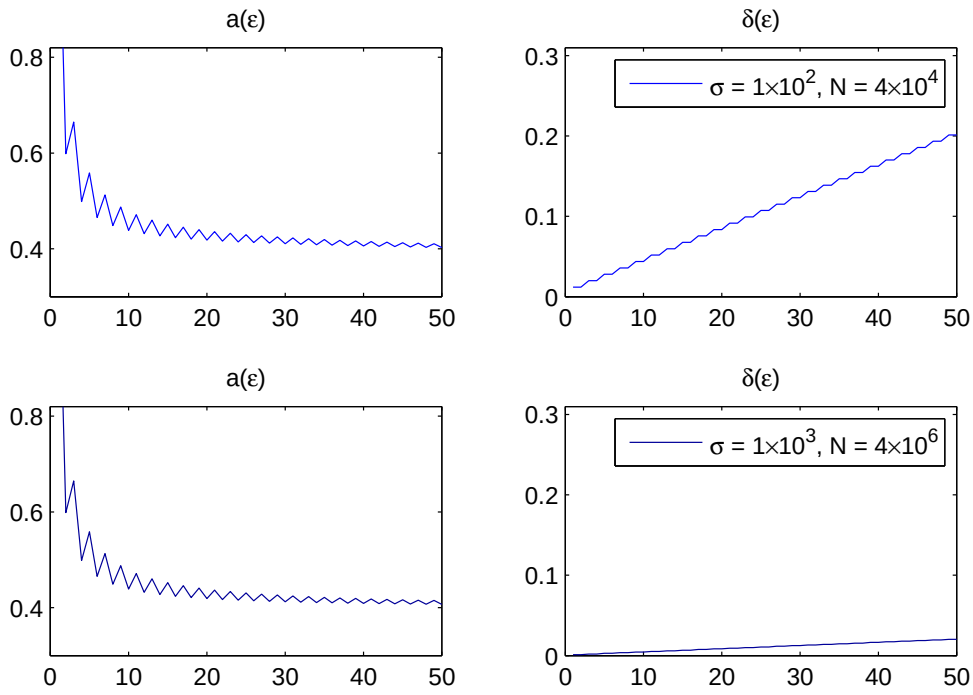

Figure 4.1: a and δ as functions of ϵ for a binomial distribution of 4×10^4 (up) and 4×10^6 (down) randomly chosen bits. Notice how the function δ takes, in a given range of ϵ, much smaller values as the number of chosen bits increases.

can fit inside an interval ϵ can be given by

$$\xi_p(\epsilon) \sim \frac{\epsilon}{\sigma}. \tag{4.12}$$

With this estimate we indeed get $a(\epsilon) \sim 1$. Figure 4.1 illustrates this for the case of a binomial distribution, where $0.2 < a(\epsilon) < 0.8$ for all $\epsilon > \frac{1}{2}$.

In general the above will work when the distribution p is approximately unimodal, i.e. characterised by a single distinct peak. If, on the contrary, the distribution was composed of two or more peaks the estimate in equation (4.12) might not hold, as Figure 4.2 exemplifies.

When (4.12) holds, taking $\epsilon \ll \sigma$ is also enough to ensure $\delta(\epsilon) \ll 1$. Note that in Figure 4.1, $a(\epsilon)$ diverges for small ϵ. To avoid such behaviour, we would typically want to choose ϵ larger than the gaps between consecutive values of the variable. Overall, we would expect to be able to find an ϵ satisfying both $a(\epsilon) \sim 1$ and $\delta(\epsilon) \ll 1$ if the distribution is

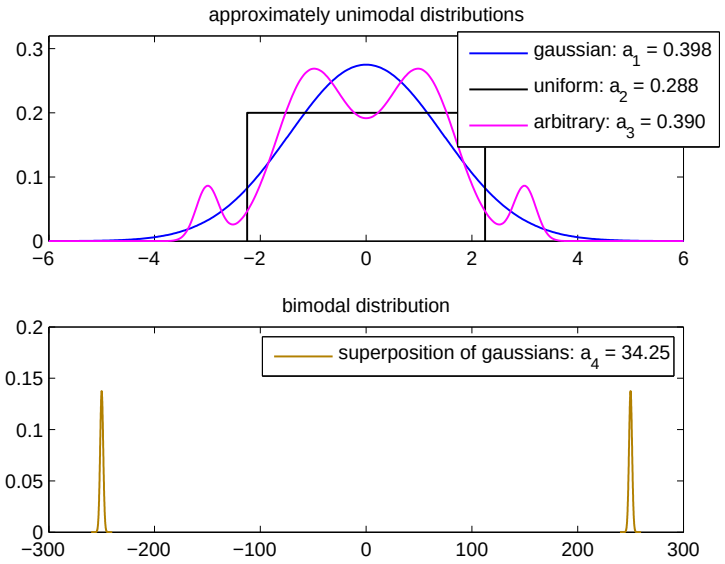

Figure 4.2: Examples of approximately unimodal distributions (above), and bimodal distribution (below), for continuous distributions in the limit $\epsilon \to 0$. The bimodal distribution can violate the estimate $\xi_p(\epsilon) \sim \frac{\epsilon}{\sigma}$, simply because one can make the standard deviation arbitrarily large by placing the peaks further apart without changing the actual value of $\xi_p(\epsilon)$.

approximately unimodal and spread over many different values of the random variable.

In our particular case, Proposition 4.1 refers to the distribution $p_\alpha = p_{(j,k)} = \frac{|\rho_{jk}||A_{kj}|}{Q\|A\|}$, which depends strongly on the distribution of energy gaps of the system. For large systems with typical energy ranges (e.g. finite positive temperatures), their energy levels tend to be more densely packed for larger energies, which leads to a much larger concentration of small gaps than large gaps. For most A and ρ_0 we would therefore expect the distribution p_α to be more peaked towards the center and decay for larger values of the energy gaps G, leading to an approximately unimodal distribution over a dense spectrum as considered above. Nevertheless, this will not always be the case, as we will see at the end of Section 4.4.2.

4.3 Observable dependent time scale bound

Propositions 4.1 and 4.2 lead to the following result.

Theorem 4.3 (Observable dependent bound)**.** *For any initial state ρ_0, observable A, Hamil-*

tonian H, and ϵ, the time averaged weak-distinguishability satisfies

$$\begin{aligned}\left\langle \widetilde{\mathcal{D}}_A(\rho_t,\omega)\right\rangle_T &\leq cQ^2\left(\frac{a(\epsilon)}{\sigma_G T}+\delta(\epsilon)\right)\\ &\leq \frac{c\|A\|^{1/2}a(\epsilon)Q^{5/2}}{T\sqrt{\left|\mathrm{Tr}\Big(\big[\,[\rho_0,H]\,,H\big]A\Big)\right|}}+c\,\delta(\epsilon)Q^2,\end{aligned} \tag{4.13}$$

where

$$Q^2 \leq d\,\mathrm{Tr}\left[\rho_0^2\right], \tag{4.14}$$

σ_G is the standard deviation of energy gaps G_α given by the distribution p_α, $a(\epsilon)$ and $\delta(\epsilon)$ are as in Proposition 4.2, $c=\frac{\pi}{1-e^{-1}}<5$, and d is the rank of ω.

Proof. Since the distribution p_α is symmetric with respect to interchanging the indices $\{j,k\}$ while G_α is antisymmetric, we get that its variance, denoted by σ_G^2, satisfies

$$\begin{aligned}\sigma_G^2 &= \sum_\alpha p_\alpha G_\alpha^2-\left(\sum_\alpha p_\alpha G_\alpha\right)^2=\sum_\alpha p_\alpha G_\alpha^2\\ &=\sum_{jk}\frac{|\rho_{jk}||A_{kj}|}{Q\|A\|}(E_j-E_k)^2\\ &\geq \frac{1}{Q\|A\|}\Big|\sum_{jk}\rho_{jk}A_{kj}(E_j-E_k)^2\Big|\\ &=\frac{1}{Q\|A\|}\Big|\mathrm{Tr}\Big(\big[\,[\rho_0,H]\,,H\big]A\Big)\Big|.\end{aligned} \tag{4.15}$$

Notice that for a local Hamiltonian and observable, and a known initial state, this expression (combined with the bound for Q which soon follows) is much simpler to compute than σ_G, since it does not require detailed knowledge of the Hamiltonian's spectrum and eigenbasis, which is needed in order to construct the distribution p_α in the first place.

Moreover, we find an upper bound for Q,

$$\begin{aligned} Q^2 &= \left(\sum_{jk:E_j \neq E_k} |\rho_{jk}| \frac{|A_{kj}|}{\|A\|} \right)^2 \\ &\leq \left(\sum_{jk} |\rho_{jk}| \frac{|A_{kj}|}{\|A\|} \right)^2 \\ &\leq \left(\sum_{jk} |\rho_{jk}|^2 \right) \left(\sum_{j'k' \in \text{ supp}(\omega)} \frac{|A_{j'k'}|^2}{\|A\|^2} \right) \\ &= \operatorname{Tr}\left[\rho_0^2\right] \frac{\operatorname{Tr}\left[\Pi_\omega A \Pi_\omega A\right]}{\|A\|^2} \\ &\leq \operatorname{Tr}\left[\rho_0^2\right] \operatorname{Tr}\left[\Pi_\omega\right] = d \operatorname{Tr}\left[\rho_0^2\right], \end{aligned} \tag{4.16}$$

where Π_ω projects onto all the energy levels of the Hamiltonian which occur with non-zero probability in ρ_0 (this is given by the support of ω). In the third line we restrict to this set of energy levels and use the Cauchy-Schwarz inequality. For the last line, notice that by the Cauchy-Schwarz inequality for the scalar product $(O, P) \equiv \operatorname{Tr}\left[O^\dagger P\right]$ we can bound $\operatorname{Tr}\left[\Pi_\omega A \Pi_\omega A\right] \leq \operatorname{Tr}\left[\Pi_\omega A^2\right]$. Then using that for any two positive semidefinite matrices $\operatorname{Tr}[OP] \leq \|O\| \operatorname{Tr}[P]$ we find $\operatorname{Tr}\left[\Pi_\omega A^2\right] \leq \operatorname{Tr}\left[\Pi_\omega\right] \|A^2\| = d\|A\|^2$.

Inserting the above into eqs. (4.3) and (4.9) proves our claim. □

The second term in eq. (4.13) needs to be small for equilibration to be possible in the first place. More precisely, given a reference equilibration constant χ (see Definition 2.9 on page 22) we need, for example, $c\,\delta(\epsilon) Q^2 \leq \chi/2$ for some value of ϵ. If this is fulfilled the system will eventually equilibrate with respect to A, since the first term tends to 0 as T grows.

The time dependence is determined by the first term. If we impose this term to also be

less than $\chi/2$, we get from Definition 2.9 that the equilibration time scale satisfies [1],

$$T_{eq} \leq \frac{2}{\chi} \frac{c\|A\|^{1/2} a(\epsilon) Q^{5/2}}{\sqrt{\left|\mathrm{Tr}\Big(\big[\,[\rho_0, H]\,, H\big] A\Big)\right|}}. \tag{4.18}$$

It is interesting to note the dependence of the above expression on $[[\rho_0, H], H]$, which is, up to a minus sign, the second time derivative of the state at $t = 0$. Therefore the bound for T_{eq} can alternatively be written as

$$T_{eq} \leq \frac{2}{\chi} \frac{c\|A\|^{1/2} a(\epsilon) Q^{5/2}}{\sqrt{\left|\,\mathrm{Tr}\left[\,\frac{d^2\rho_t}{dt^2}\Big|_{t=0} A\right]\,\right|}}. \tag{4.19}$$

Remarkably, the denominator of this expression is what one would expect from a Taylor expansion for short times, assuming the system is initially as far from equilibrium as possible (then the first derivative term is 0 and one is left with the second derivative as leading order).

We argued earlier that we would typically expect $a(\epsilon) \sim 1$ and $\delta(\epsilon) \ll 1$. However, we still have to address the size of the bound for Q given by eq. (4.14), which could greatly influence the speed of equilibration. Notice that in general the dimension d of the Hilbert space is extremely large, since it scales exponentially with the number of constituents of the closed system being considered. Therefore, in order for this bound to show rapid equilibration we would need a very mixed initial state, spread over a significant fraction of the Hilbert space. Moreover, the constant Q appears in the second term in Theorem 4.3, along with $\delta(\epsilon)$. In order to show equilibration at all this second term needs to be small too.

In the next section we consider an important physical scenario and then use our bound to show fast equilibration.

[1] As a matter of fact, notice that in the derivation of eq. (4.15) one can replace ρ_0 by the state at an arbitrary time ρ_τ, since it is the modulus of the the state's matrix elements that appear. With this a tighter bound can be obtained, giving

$$T_{eq} \leq \min_{\tau} \frac{2}{\chi} \frac{c\|A\|^{1/2} a(\epsilon) Q^{5/2}}{\sqrt{\left|\mathrm{Tr}\Big(\big[\,[\rho_\tau, H]\,, H\big] A\Big)\right|}}. \tag{4.17}$$

4.4 System interacting with a bath

We now turn to the paradigmatic case of a small system interacting with a large thermal bath. This situation corresponds to decomposing the closed system considered in the previous sections into a small system $\mathcal{S}$ and a bath $\mathcal{B}$. By assuming the observable A to be of the form

$$A = A_S \otimes \mathbb{1}_B, \tag{4.20}$$

where A_S acts on the system and $\mathbb{1}_B$ is the identity acting on the bath, one can focus on the system's behaviour.

The total Hamiltonian is denoted by

$$H = H_S + H_B + H_I, \tag{4.21}$$

where H_S and H_B are the system and bath Hamiltonians, and H_I denotes the interaction between them.

We assume that the system $\mathcal{S}$ is initially in an arbitrary state ρ_S, and for simplicity not correlated with the initial state of bath ρ_B, that is $\rho_0 = \rho_S \otimes \rho_B$, corresponding to a system initially isolated which is suddenly allowed to interact with $\mathcal{B}$ via H_I.

To show that such a situation can lead to a small value for Q, we first consider the case in which the bath is in a maximally mixed state (which could be understood as a system interacting with an infinite temperature bath), with

$$\rho_0 = \rho_S \otimes \frac{\mathbb{1}_B}{d_B}. \tag{4.22}$$

In this case, it is easy to see from equation (4.14) that

$$Q \leq d \operatorname{Tr}\left[\rho_0^2\right] \leq (d_S d_B) \operatorname{Tr}_S\left[\rho_S^2\right] \operatorname{Tr}_B\left[\frac{\mathbb{1}_B^2}{d_B^2}\right] = d_S \operatorname{Tr}_S\left[\rho_S^2\right]. \tag{4.23}$$

The remainder of this section is devoted to extending our results to the more physical case of a system interacting with a finite temperature bath.

In what follows, given a Hamiltonian H we denote an energy window of width Δ centered

around an energy E in terms of its corresponding Hilbert space $\mathcal{H}_H^{E,\Delta}$, defined as

$$\mathcal{H}_H^{E,\Delta} = \text{span}\left\{|E_j\rangle \,:\, E - \frac{\Delta}{2} \leq E_j \leq E + \frac{\Delta}{2}\right\}. \tag{4.24}$$

We will consider the state of the bath from the microcanonical ensemble viewpoint. Consequently, we consider an energy window of the bath Hamiltonian of width Δ centered around E_B. The subspace that this defines, $\mathcal{H}_{H_B}^{E_B,\Delta}$, will be referred to as a *microcanonical window*, and its dimension will be denoted by d_B^Δ. The width of this window is to be taken large enough such that it contains many energy levels, in particular many more than the dimension of the system, yet small in comparison to the whole spectrum of the bath Hamiltonian H_B.

Thus, the initial state of the bath is given by $\rho_B = \frac{\mathbb{1}_B^\Delta}{d_B^\Delta}$, and the initial state of the system plus bath is

$$\rho_0 = \rho_S \otimes \frac{\mathbb{1}_B^\Delta}{d_B^\Delta}, \tag{4.25}$$

which we will use from now on.

4.4.1 Truncation of the Hilbert space

Notice that the state $\rho_0 = \rho_S \otimes \frac{\mathbb{1}_B^\Delta}{d_B^\Delta}$, corresponding to a bath in the microcanonical ensemble, is quite mixed. This is good news for our bound $Q^2 \leq d\,\text{Tr}\left[\rho_0^2\right]$ given by equation (4.14), since the purity of the state will be a small number. However, the presence of the dimension of the Hilbert space implies that the bound for Q could still be extremely large. In this section we show a truncation method for the state and the Hilbert space which allows us to reduce the relevant dimension significantly.

As the eigenvalues of H_S lie between $-\|H_S\|$ and $\|H_S\|$, the initial state ρ_0 is contained inside an energy window of width $\Delta + 2\|H_S\|$ of the unperturbed Hamiltonian $H_S + H_B$. That is, ρ_0 lies within the subspace $\mathcal{H}_{H_B+H_S}^{E_B,\Delta+2\|H_S\|}$.

However, this no longer holds when considering the full Hamiltonian $H = H_S + H_B + H_I$; in principle ρ_0 can have support outside the subspace $\mathcal{H}_{H_B+H_S+H_I}^{E_B,\Delta+2\|H_S\|}$. Yet, one has the intuition that if the interaction is small compared to the unperturbed Hamiltonian the energy window where the state is supported should not grow significantly. This would imply that one does

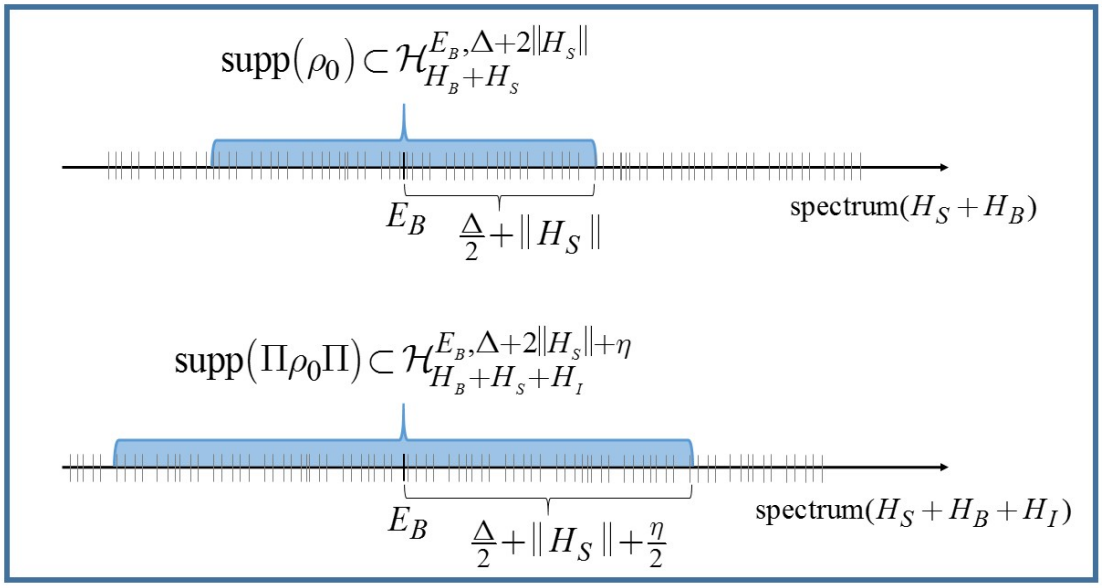

Figure 4.3: The support of the state $\rho_0 = \rho_S \otimes \frac{\mathbb{1}_B^{\Delta}}{d_B^{\Delta}}$ is contained in the Hilbert space $\mathcal{H}^{E_B,\Delta+2\|H_S\|}_{H_B+H_S}$, depicted above. However, the inclusion of the interaction Hamiltonian takes the state out of the original window. We prove in Proposition 4.6 that the state can be truncated to $\Pi\rho_0\Pi$, supported inside the Hilbert space $\mathcal{H}^{E_B,\Delta+2\|H_S\|+\eta}_{H_B+H_S+H_I}$, which we depict below. The error introduced by the truncation procedure is small as long as the extra width η of the truncation window is taken large enough.

not need to consider the full Hilbert space, but rather a truncated subspace corresponding to a window somewhat larger than the original $\mathcal{H}^{E_B,\Delta+2\|H_S\|}_{H_B+H_S}$ (see Figure 4.3 for an illustration of this truncation procedure).

We will show that the above reasoning is correct, by proving that the trace distance between the state ρ_0 and a truncated state $\Pi\rho_0\Pi$ is small, where Π is a projector onto the truncated subspace. In order to prove this, we will use the two following results.

Lemma 4.4 (Gentle measurement [86])**.** *For any state ρ and positive operator X such that $X \leq 1$ and*

$$1 - \mathrm{Tr}\left[\rho X\right] \leq \frac{1}{2K^2} \leq 1, \tag{4.26}$$

one has

$$\|\rho - \sqrt{X}\rho\sqrt{X}\|_1 \leq \frac{2}{K}. \tag{4.27}$$

The second one is a result related to perturbation theory, which can be found in [87] (Theorem VII.3.1)[2].

Theorem 4.5 (Bhatia)**.** *Let O and P be normal operators, S_1 and S_2 be two subsets of the complex plane that are separated by a strip (or annulus) of width Δ, and let E (F) denote the orthogonal projection onto the subspace spanned by the eigenvectors of O (P) corresponding to those of its eigenvalues that lie in S_1 (S_2). Then, for every unitarily invariant norm $|||\cdot|||$,*

$$|||EF||| \leq \frac{|||O-P|||}{\Delta}. \tag{4.28}$$

Truncating the Hilbert space

With the above tools in hand, we prove the following.

Proposition 4.6 (Hilbert space truncation)**.** *For any K, the state $\rho_0 = \rho_S \otimes \frac{\mathbb{1}_B^\Delta}{d_B^\Delta}$ which lies within $\mathcal{H}_{H_B+H_S}^{E_B,\Delta+2\|H_S\|}$ can be truncated to the state $\Pi\rho_0\Pi$, with*

$$\|\rho_0 - \Pi\rho_0\Pi\|_1 \leq \frac{2}{K}, \tag{4.29}$$

where Π projects onto the subspace $\mathcal{H}_{H_B+H_S+H_I}^{E_B,\Delta+2\|H_S\|+\eta}$ with a width extended by $\eta = \sqrt{8d_S}\|H_I\|K$.

Proof. We want to show that, when considering the full interacting Hamiltonian $H = H_S + H_B + H_I$, it is enough to consider the truncated subspace $\mathcal{H}_{H_S+H_B+H_I}^{E_B,\Delta+2\|H_S\|+\eta}$, where η denotes the amount by which the energy window is extended.

The effect of "cutting" the state outside the space $\mathcal{H}_{H_S+H_B+H_I}^{E_B,\Delta+2\|H_S\|+\eta}$ will obviously introduce errors. We wish to do it such that the truncated state remains close to the original one in trace distance:

$$\|\rho_0 - \Pi\rho_0\Pi\|_1 \leq \frac{2}{K}, \tag{4.30}$$

where Π is the projector onto $\mathcal{H}_{H_B+H_S+H_I}^{E_B,\Delta+2\|H_S\|+\eta}$ and $\eta = \sqrt{8d_S}\|H_I\|K$.

[2]For another interesting and related application of Bhatia's theorem, treating the problem of proving thermalization in closed quantum systems, see [44].

An arbitrary initial state of the system can be written as

$$\rho_S = \sum_{l,l'} \rho^S_{ll'} \left|E^S_l\right\rangle \left\langle E^S_{l'}\right|, \tag{4.31}$$

where $\left|E^S_l\right\rangle$ are eigenvectors of H_S with energy E^S_l. Since the state of the bath is proportional to the identity onto a window of H_B, and therefore diagonal in the basis H_B, we can write the total state as

$$\begin{aligned}\rho_0 &= \sum_{\lambda} \sum_{l,l'} c_\lambda \rho^S_{ll'} \left|E^S_l\right\rangle \left\langle E^S_{l'}\right| \otimes \left|E^B_\lambda\right\rangle \left\langle E^B_\lambda\right| \\ &\equiv \sum_{\lambda,l,l'} c_\lambda \rho^S_{ll'} \left|E^S_l, E^B_\lambda\right\rangle \left\langle E^S_{l'}, E^B_\lambda\right|, \end{aligned} \tag{4.32}$$

where $\left|E^B_\lambda\right\rangle$ are the eigenvectors of H_B and the coefficients c_λ are positive and normalized (we will do the calculation for an arbitrary state of the bath commuting with H_B, but in our case actually $c_\lambda = 1/d_B^\Delta$).

By defining $\Pi^\perp \equiv \mathbb{1} - \Pi$, taking absolute values in line 3, and in line 4 using the Cauchy-Schwarz inequality (with $\| \left|\psi\right\rangle \| = \sqrt{\langle\psi|\psi\rangle}$ as usual), we see

$$\begin{aligned} 1 - \mathrm{Tr}\left[\rho_0 \Pi\right] &= \mathrm{Tr}\left[\rho_0 \Pi^\perp\right] \\ &= \sum_{\lambda,l,l'} c_\lambda \rho^S_{ll'} \,\mathrm{Tr}\left[\left|E^S_l, E^B_\lambda\right\rangle \left\langle E^S_{l'}, E^B_\lambda\right| \Pi^\perp\right] \\ &\leq \sum_{\lambda,l,l'} c_\lambda \left|\rho^S_{ll'}\right| \left|\left\langle E^S_{l'}, E^B_\lambda\right| \Pi^\perp \left|E^S_l, E^B_\lambda\right\rangle\right| \\ &\leq \sum_{\lambda,l,l'} c_\lambda \left|\rho^S_{ll'}\right| \left\|\Pi^\perp \left|E^S_l, E^B_\lambda\right\rangle\right\| \left\|\Pi^\perp \left|E^S_{l'}, E^B_\lambda\right\rangle\right\|. \end{aligned} \tag{4.33}$$

In our notation, Bhatia's Theorem 4.5 on page 61 implies

$$\left\|\Pi^\perp \left|E^S_l, E^B_\lambda\right\rangle\right\| = \left\|\Pi^\perp \left|E^S_l, E^B_\lambda\right\rangle \left\langle E^S_l, E^B_\lambda\right|\right\| \leq \frac{\|H_I\|}{\Delta_{l,\lambda}}, \tag{4.34}$$

where we have related the euclidean vector norm on the left to the operator norm on the right. In the above expression $\Delta_{l,\lambda}$ is the distance between the supports of $\left|E^S_l, E^B_\lambda\right\rangle \left\langle E^S_l, E^B_\lambda\right|$ and $\Pi^\perp$. Note that this distance satisfies $\Delta_{l,\lambda} \geq \frac{\eta}{2}$.

Using equations (4.33) and (4.34), the fact that for a system in an arbitrary initial state

$$\left(\sum_{l,l'}|\rho^S_{ll'}|\right)^2 \leq d_S^2 \sum_{l,l'}|\rho^S_{ll'}|^2 = d_S^2 \operatorname{Tr}\left[\rho_S^2\right] \leq d_S^2, \tag{4.35}$$

and $\sum_\lambda c_\lambda = 1$, we get

$$\begin{aligned} 1 - \operatorname{Tr}\left[\rho_0 \Pi\right] &\leq \sum_{\lambda,l,l'} c_\lambda \left|\rho^S_{ll'}\right| \frac{4\|H_I\|^2}{\eta^2} \\ &\leq d_S \frac{4\|H_I\|^2}{\eta^2}. \end{aligned} \tag{4.36}$$

We can now apply Lemma 4.4 on page 60 for the state $\rho = \rho_0$ and the operator $X = \sqrt{X} = \Pi$. Choosing the truncation window with $\eta = K\sqrt{8d_S}\|H_I\|$ leads to the main result

$$\|\rho_0 - \Pi\rho_0\Pi\|_1 \leq \frac{2}{K}. \tag{4.37}$$

□

Notice that if the system is in equilibrium before the interaction with the bath (i.e. if $[\rho_S, H_S] = 0$), eq. (4.35) turns into $\left(\sum_{l,l'}|\rho^S_{ll'}|\right)^2 = 1$, which gives a tighter result with $\eta* = K\sqrt{8}\|H_I\|$.

The weak-distinguishability after the truncation

The following is a straightforward consequence of Proposition 4.6.

Corollary 4.7 (Weak distinguishability after the truncation)**.** *The evolved state $\rho_t = e^{-iHt}\rho_0 e^{iHt}$, with $\rho_0 = \rho_S \otimes \frac{\mathbb{1}_B^\Delta}{d_B^\Delta}$, can be truncated to the state $\Pi\rho_t\Pi$ contained in the subspace $\mathcal{H}^{E_B,\Delta+2\|H_S\|+\eta}_{H_B+H_S+H_I}$, with*

$$\mathcal{D}_A\left(\rho_t, \Pi\rho_t\Pi\right) \leq \frac{1}{K^2}. \tag{4.38}$$

Proof. Note that the trace distance is invariant under global unitaries, in particular invariant under the Hamiltonian evolution. Therefore, expectation values of an observable A will be

close, since we have

$$\begin{aligned} |\mathrm{Tr}\left[A\rho_t\right] - \mathrm{Tr}\left[A\Pi\rho_t\Pi\right]| &\leq \|\rho_t - \Pi\rho_t\Pi\|_1\|A\| \\ &= \|\rho_0 - \Pi\rho_0\Pi\|_1\|A\| \\ &\leq \frac{2\|A\|}{K}, \end{aligned} \tag{4.39}$$

by using in the first step that for any two operators O and P Holder's inequality implies $\mathrm{Tr}\left[OP\right] \leq \|OP\|_1 \leq \|O\|_1\|P\|$. This equation and the definition of the weak-distinguishability finishes the proof. □

This corollary shows that, as long as we take the truncation window such that K is large enough, the two states give similar evolutions according to the figure of merit implied by the weak-distinguishability. Hence, we are free to use the truncated Hilbert space $\mathcal{H}_{H_B+H_S+H_I}^{E_B,\Delta+2\|H_S\|+\eta}$ (along with the truncated states) instead of the full original space $\mathcal{H}$.

Dimension of the truncated space

This truncation procedure will be particularly useful to us, since as we now see the dimension of the accessible Hilbert space $\mathcal{H}_{H_B+H_S+H_I}^{E_B,\Delta+2\|H_S\|+\eta}$ is in general much smaller than the full dimension.

Proposition 4.8 (Dimension of the truncated space)**.** *Let $\nu_B(E)$ denote the density of states of the bath. Then the dimension of the truncated state satisfies*

$$d_{trunc} \leq \frac{d_S}{1-\frac{1}{K}} \int_{E_B-\frac{\Delta}{2}-\left(1+\sqrt{2d_s}\right)K\|H_I\|-\|H_S\|}^{E_B+\frac{\Delta}{2}+\left(1+\sqrt{2d_s}\right)K\|H_I\|+\|H_S\|} \nu_B(E)dE. \tag{4.40}$$

Proof. It will be useful to relate the dimension of the truncated space $\mathcal{H}_{H_B+H_S+H_I}^{E_B,\Delta+2\|H_S\|+\eta}$ (i.e. the rank of Π) to the rank of a projector P onto yet another extended subspace $\mathcal{H}_{H_B+H_S}^{E_B,\Delta+2\|H_S\|+\eta+\eta'}$. Since the rank of P is related to the spectrum of unperturbed system and bath Hamiltonians it will prove simpler to calculate.

First, denoting the orthogonal projector of P by $P^{\perp}$, we get

$$\begin{aligned}\|\Pi - \Pi P\|_1 &= \|\Pi P^{\perp}\|_1 \\ &\leq \operatorname{rank}(\Pi)\, \|\Pi P^{\perp}\| \\ &\leq \|\Pi\|_1 \frac{2\|H_I\|}{\eta'} = \frac{\|\Pi\|_1}{K},\end{aligned} \tag{4.41}$$

by using that for any operator $\|Q\|_1 \leq \operatorname{rank}(Q)\, \|Q\|$, Bhatia's Theorem 4.5 on page 61, and setting $\eta' = 2K\|H_I\|$. The triangle inequality then leads to

$$\begin{aligned}\|\Pi\|_1 &\leq \|\Pi P\|_1 + \|\Pi - \Pi P\|_1 \\ &\leq \|P\|_1 + \frac{\|\Pi\|_1}{K}.\end{aligned} \tag{4.42}$$

Recall that $d_{\text{trunc}} = \operatorname{rank}(\Pi) = \|\Pi\|_1$. Hence

$$d_{\text{trunc}} \leq \frac{\|P\|_1}{1 - \frac{1}{K}}. \tag{4.43}$$

Note that, since P projects onto the subspace $\mathcal{H}_{H_B+H_S}^{E_B,\Delta+2\|H_S\|+\eta+\eta'}$ corresponding to a system that does not interact with the bath, we can denote the density of states of the bath by $\nu_B(E)$, and

$$\begin{aligned}\|P\|_1 &\leq d_S \int_{E_B - \frac{\Delta}{2} - \frac{\eta}{2} - \frac{\eta'}{2} - \|H_S\|}^{E_B + \frac{\Delta}{2} + \frac{\eta}{2} + \frac{\eta'}{2} + \|H_S\|} \nu_B(E) dE \\ &= d_S \int_{E_B - \frac{\Delta}{2} - \left(1+\sqrt{2d_s}\right)K\|H_I\| - \|H_S\|}^{E_B + \frac{\Delta}{2} + \left(1+\sqrt{2d_s}\right)K\|H_I\| + \|H_S\|} \nu_B(E) dE.\end{aligned} \tag{4.44}$$

The inequality comes from upper bounding the number of accessible states of the system by d_S, and counting the states of the bath as if it could access all of the possible energies of the space $\mathcal{H}_{H_B+H_S}^{E_B,\Delta+\|H_S\|+\eta+\eta'}$. The second line comes from using $\eta' = 2K\|H_I\|$ and $\eta = \sqrt{8d_S}K\|H_I\|$.

□

Meanwhile, the dimension of the (unperturbed) microcanonical window of the bath is

given by

$$d_B^{\Delta} = \int_{E_B - \frac{\Delta}{2}}^{E_B + \frac{\Delta}{2}} \nu_B(E) dE. \tag{4.45}$$

Typically, thermal baths have a (coarse grained) density of states which grows approximately exponentially with energy, and in such case the following corollary gives the dimension of the truncated space.

Corollary 4.9 (Dimension of truncated space for a thermal bath)**.** *For a thermal bath with a density of states given by*

$$\nu_B(E) = \mathcal{N} e^{\beta E}, \tag{4.46}$$

where β is the inverse temperature and $\mathcal{N}$ a normalization constant,

$$d_{trunc} \leq \frac{d_S d_B^{\Delta}}{\left(1 - \frac{1}{K}\right)\left(1 - e^{-\beta\Delta}\right)} e^{\beta\|H_S\| + \left(1+\sqrt{2d_s}\right) K\beta\|H_I\|}. \tag{4.47}$$

Proof. The proof comes from a straightforward application of Proposition 4.8,

$$\begin{aligned} d_{\text{trunc}} &\leq \frac{d_S d_B^{\Delta}}{\left(1 - \frac{1}{K}\right)} \frac{\sinh\left[\beta\frac{\Delta}{2} + \beta\|H_S\| + \left(1 + \sqrt{2d_s}\right) K\beta\|H_I\|\right]}{\sinh\left[\beta\frac{\Delta}{2}\right]} \\ &\leq \frac{d_S d_B^{\Delta}}{\left(1 - \frac{1}{K}\right)\left(1 - e^{-\beta\Delta}\right)} e^{\beta\|H_S\| + \left(1+\sqrt{2d_s}\right) K\beta\|H_I\|}. \end{aligned} \tag{4.48}$$

□

Note that, given that the energy width of the microcanonical window grows as the number of constituents of the bath increases, in general $\beta\Delta \gg 1$ holds for a large enough bath, in which case the last inequality is a particularly good approximation.

4.4.2 Time scales for a system in contact with a bath

Proposition 4.6 on page 61 allows to truncate the microcanonical state ρ_0 to $\Pi\rho_0\Pi$, since the error introduced is small. This greatly reduces the dimension of the relevant Hilbert space, and consequently the corresponding bound for the constant Q in Theorem 4.3 on page 54.

However, strictly speaking the above reasoning would lead us to conclude that the truncated state should appear when revisiting the theorem. This would not be the most desirable situation since calculating the factor $\mathrm{Tr}\Big(\left[[\Pi\rho_0^{mc}\Pi, H], H\right] A\Big)$ in eq. (4.13) on page 55 would not be straightforward. This not only introduces additional complexity but could possibly significantly weaken the bound. Moreover, even if the Hamiltonian involved nearest neighbour-type interactions, Π could be highly non-local and indeed we may have no way of computing it. Nevertheless, we can prove that the time average of the weak-distinguishability can be bounded with a commutator involving the original state ρ_0 instead of the truncated one, while still having a relevant Hilbert space with much smaller dimension than the original space (we leave the details of this proof for Appendix A.2 on page 99).

This gives all the ingredients necessary to apply Theorem 4.3 to the case of a system in contact with a thermal bath, which turns into the following.

Theorem 4.10 (Bound for system interacting with thermal bath)**.** *For any ϵ and K, observable A, and Hamiltonian $H = H_B + H_S + H_I$, the weak-distinguishability satisfies*

$$\left\langle \widetilde{\mathcal{D}}_A\left(\rho_t, \omega\right)\right\rangle_T \leq \frac{c\|A\|^{1/2} a(\epsilon) Q_2^{5/2}}{T\sqrt{\left|\mathrm{Tr}\Big(\left[\left[\rho_0, H\right], H\right] A\Big)\right|}} + c\,\delta(\epsilon) Q_2^2 + \frac{18}{K^2}, \tag{4.49}$$

where

$$Q_2 \leq \sqrt{\mathrm{Tr}\left[\rho_0^2\right] d_{\mathrm{trunc}}} + \frac{2}{K}, \tag{4.50}$$

$a(\epsilon)$ and $\delta(\epsilon)$ are as in Proposition 4.2, $c = \frac{\pi}{1-e^{-1}} < 5$, and $\rho_0 = \rho_S \otimes \frac{\mathbb{1}_B^{\Delta}}{d_B^{\Delta}}$.

Moreover, if the bath has an approximately exponentially increasing density of states we obtain from Corollary 4.9 on page 66 that

$$Q_2 \leq \sqrt{\frac{d_S\,\mathrm{Tr}_S\left[\rho_S^2\right]\, e^{\beta\|H_S\| + \left(1+\sqrt{2d_s}\right)K\beta\|H_I\|}}{\left(1-\frac{1}{K}\right)\left(1-e^{-\beta\Delta}\right)}} + \frac{2}{K}. \tag{4.51}$$

Note that if the system is in equilibrium before the interaction with the bath, i.e. if $[\rho_S, H_S] = 0$, the factor $\sqrt{d_S}$ in the exponent does not appear (see comment after the proof of Proposition 4.6 on page 61).

Let us focus more closely on this result. Firstly, all time independent terms have to be small for our theorem to imply equilibration in the first place. The factors involving K in equations (4.49) and (4.51) come from the truncation procedure, and are small as long the microcanonical window and the truncation window are large enough.

The other time independent term is $c\,\delta(\epsilon)Q_2^2$, which we have neglected so far. As discussed in Section 4.2, for distributions p_α that are approximately unimodal and sufficiently spread over different values one can estimate that $\delta(\epsilon) \sim \frac{\epsilon}{\sigma_G}$. Notice that as the bath grows in size one would expect that this holds for smaller values of ϵ, since the distribution p_α would be spread over more values. We could therefore take ϵ smaller and smaller and reduce $\delta(\epsilon)$. At the same time, the bound on Q_2 in equation (4.51) will generally not grow with the dimension of the bath. To see this note that typically (e.g. for short range interactions in a lattice system), $\|H_I\|$ will not increase significantly as the bath size increases, and that increasing the width Δ of the microcanonical window as the bath grows will cause the bound to become tighter. Therefore, in the limit of increasing bath sizes the term $c\,\delta(\epsilon)Q_2^2$ becomes negligible, as needed.

The fact that the results in Theorem 4.10 do not depend on the dimension of the full Hilbert space is a very noticeable aspect of this work [3]. This is in stark contrast with previously know general upper bounds on the time scale of equilibration, which essentially scale with the full Hilbert space dimension as we explained in Section 2.3.2 on page 23.

Finally, the first term in (4.49) determines the time decay of the weak-distinguishability, and can be interpreted the same way as in the corresponding term in Theorem 4.3 on page 54 (see subsequent discussion). Notice that, once $a(\epsilon)$ is estimated, the time dependence can in general be calculated analytically for a given initial state, Hamiltonian and observable. Moreover, performing this calculation is much simpler than solving the exact time evolution, which involves commutators of initial state and Hamiltonian of all orders and can only be done for simple models.

It is illuminating to ask how our bound behaves in a case where no equilibration occurs. Take, for example, a spin 1/2 in a pure initial state $|\Psi\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle + |\downarrow\rangle\right)$ as the system $\mathcal{S}$, and a bath composed of N other spins in the microcanonical ensemble. Furthermore, take

[3] Notice that for $A = A_S \otimes \mathbb{1}_B$ the denominator of the first term does not scale with the size of the bath either, since in such a case $\mathrm{Tr}\left[\rho_0\left[H,[H,A]\right]\right] = \mathrm{Tr}\left[\rho_0\left[H_S+H_I,[H_S+H_I,A_S\otimes\mathbb{1}_B]\right]\right]$.

the Hamiltonian $H = \Omega\sigma_z^S + H_B$, and the observable $A = \sigma_x^S \otimes \mathbb{1}_B$. Since the system does not interact with the bath it does not equilibrate with respect to the observable A. The key to understanding where our bound expresses this fact is in the factor $\delta(\epsilon)$. It is easy to see that the distribution p_α is composed of only 2 values, corresponding to the gaps Ω and $-\Omega$, which results in $\delta(\epsilon) \geq \frac{1}{2}$ for any ϵ, hence no equilibration at all.

The distribution p_α for a spin ring

In order to get a deeper grasp of the behaviour of p_α, we simulated L interacting spin 1/2's, with a Hamiltonian given by

$$H = \Omega \sum_{\lambda=1}^{L} \sigma_\lambda^z + \gamma\Omega \sum_{\lambda=1}^{L} \sigma_\lambda^x \sigma_{\lambda+1}^x, \tag{4.52}$$

where σ_λ^z and σ_λ^x are the Pauli z and x operators for the spin λ, and we adopt the notation $\sigma_{L+1}^x = \sigma_1^x$. The spin $\lambda = 1$ is taken to represent the system $\mathcal{S}$, and we focus on an observable and initial state given by

$$A = \sigma_1^x \bigotimes_{\lambda=2}^{L} \mathbb{1}_\lambda, \qquad \rho_0 = |1\rangle\langle 1| \bigotimes_{\lambda=2}^{L} \frac{\mathbb{1}_\lambda}{2}, \tag{4.53}$$

where $|1\rangle$ is the eigenvector of σ_1^z with eigenvalue 1. Figure 4.4 depicts the behaviour of the distribution p_α as the interaction strength increases, illustrating the transition between a distribution with several distinct peaks and a unimodal distribution, for which an ϵ can be taken such that $a(\epsilon) \sim 1$ and $\delta(\epsilon) \ll 1$. In Figure 4.5 the interaction strength is fixed, and the size of the system is gradually increased. For completeness, we include the Matlab script used for the simulation in Appendix A.2.4.

4.4.3 Environment in a pure state: the typical behaviour

So far we have considered mixed initial states of the total closed system. Here we show that our results can be extended to the typical behaviour of pure initial states of the environment that interacts with the system.

Let us consider the environment's initial state to be pure, and drawn at random from the

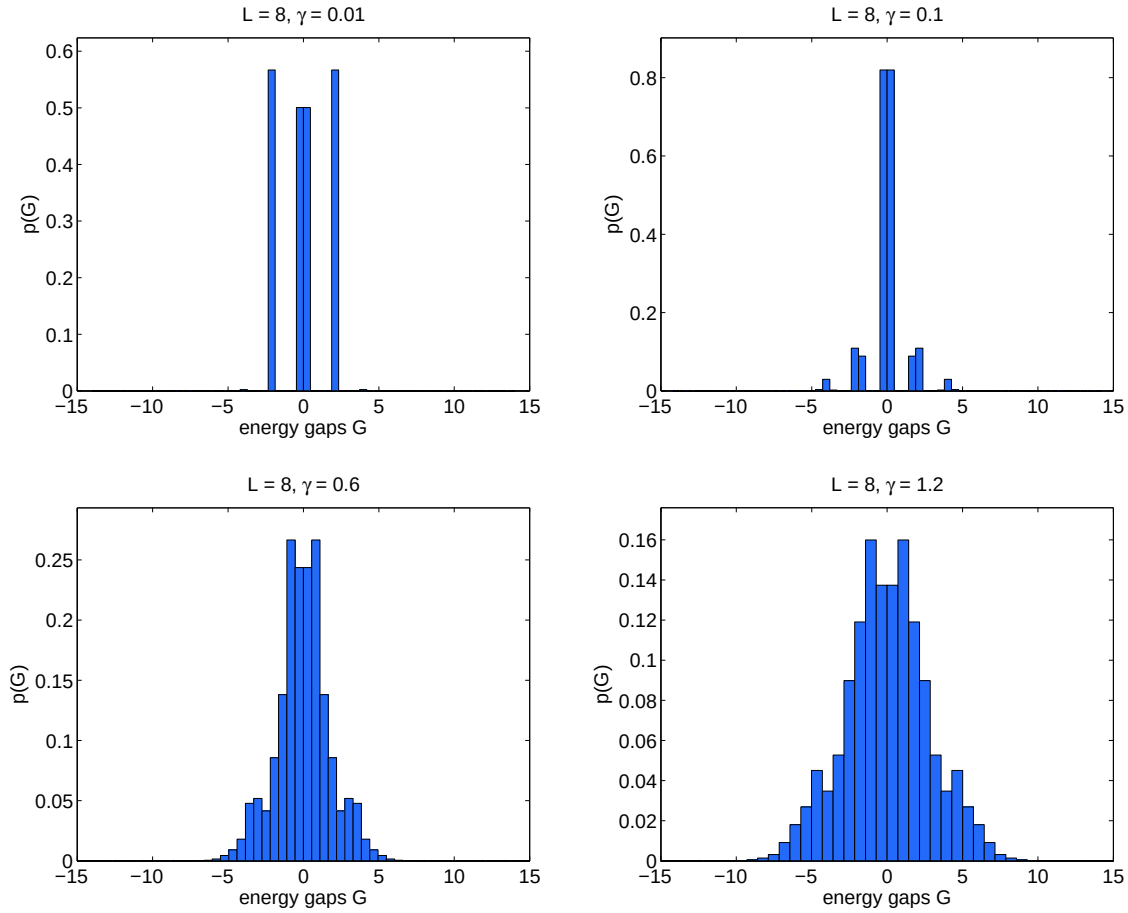

Figure 4.4: Normalized histogram of the distribution p_α as a function of the energy gaps for a spin ring composed of $L = 8$ spins, for different values of the interaction strength γ. For small interaction strengths the distribution is composed of distinct peaks. As γ increases the function becomes more unimodal, while at the same time the value of $\delta(\epsilon)$ (the maximum probability that fits an interval of length ϵ) decreases, for a given ϵ. For small or no interaction there is no ϵ such that $\delta(\epsilon)$ is significantly small, meaning that no equilibration is derived by Theorem 4.10 (as should be, since in such a case equilibration is extremely slow or does not occur).

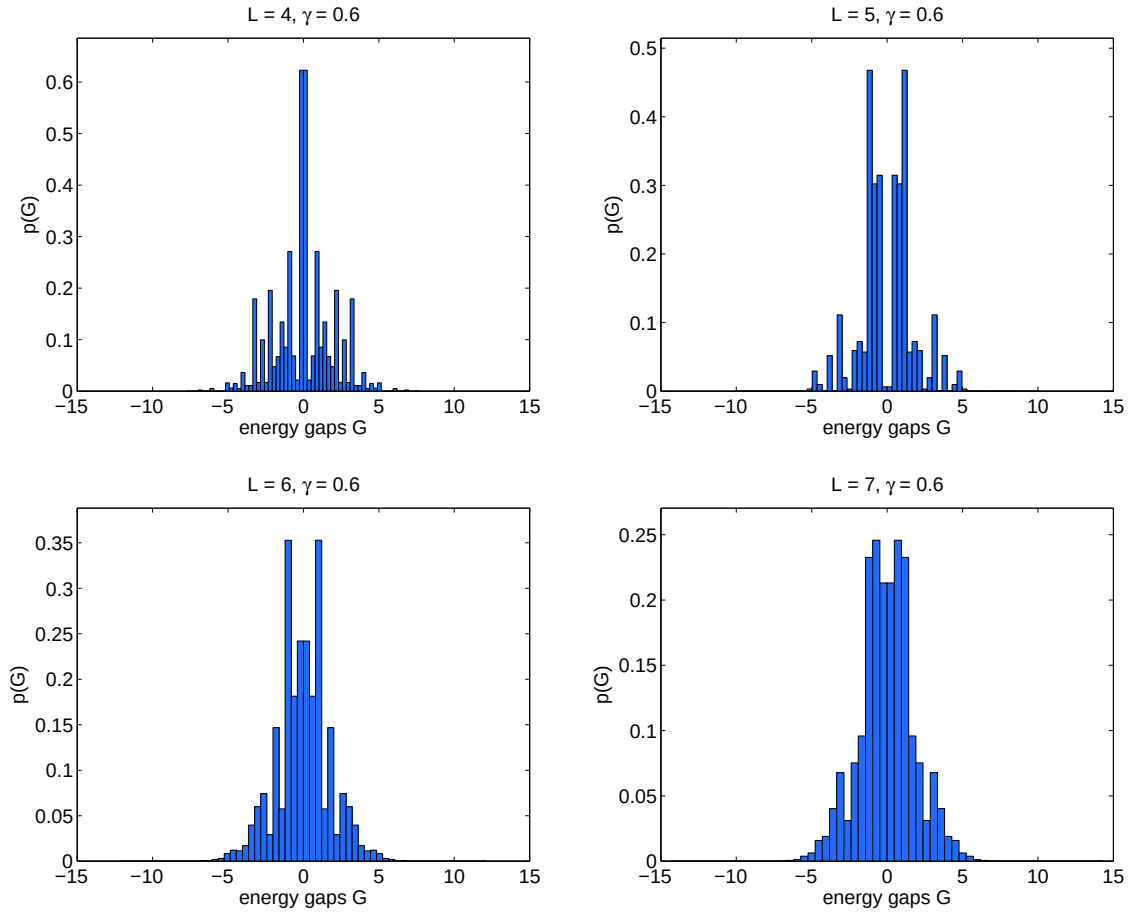

Figure 4.5: Normalized histogram of the distribution p_α as a function of the energy gaps for a spin ring, for different number of spins L. The function p_α is spread over more values as the size of the system increases. At the same time, as L increases the distribution becomes more distinctly unimodal.

microcanonical window. Any pure state from the microcanonical window can be written as

$$\rho_B^U = U \left|\psi\right\rangle \left\langle\psi\right| U^\dagger, \tag{4.54}$$

where U is a unitary operator acting on $\mathcal{H}_{H_B}^{E_B,\Delta}$. By averaging over all possible U's, drawn from the Haar measure, we have the typical behavior for random pure states from the microcanonical subspace $\mathcal{H}_{H_B}^{E_B,\Delta}$.

It turns out that taking the environment state at random from a microcanonical window is equivalent to the environment starting in the maximally mixed state $\frac{\mathbb{1}_B^\Delta}{d_B^\Delta}$, where $\mathbb{1}_B^\Delta$ is the identity over $\mathcal{H}_{H_B}^{E_B,\Delta}$. More precisely, we show in Appendix A.3 on page 107 the following.

Proposition 4.11 (Evolution for typical initial states of the bath)**.** *The weak-distinguishability averaged over all possible initial pure states of the environment drawn from a microcanonical window of width Δ satisfies*

$$\left\langle \widetilde{\mathcal{D}}_A\big(\rho_t^U, \omega^U\big)\right\rangle_U \leq \widetilde{\mathcal{D}}_A\big(\rho_t, \omega\big) + \frac{d_S}{d_B^\Delta},$$

where $\rho_0^U = \rho_S \otimes U \left|\psi\right\rangle \left\langle\psi\right| U^\dagger$ with corresponding evolved and equilibrium states ρ_t^U and ω^U, and $\rho_0 \equiv \rho_S \otimes \frac{\mathbb{1}_B^\Delta}{d_B^\Delta}$ with corresponding evolved and equilibrium states ρ_t and ω.

Since the microcanonical window is assumed to contain a lot more levels than the system's dimension, $d_B^\Delta \gg d_S$, the above expression implies that for typical initial pure states of the bath the evolution is as if the initial state was $\rho_0 = \rho_S \otimes \frac{\mathbb{1}_B^\Delta}{d_B^\Delta}$.

It is straightforward to combine this proposition with Theorem 4.10 and show that the upper bound for the typical time scale of equilibration for a system interacting with an environment in a pure state is the same as if the environment were in the microcanonical state.

4.5 Discussion

From Chapter 3 we know that one needs to impose further conditions in order to prove reasonably fast equilibration, since extremely slow observables can always be constructed.

In this chapter we have found a set of sufficient conditions that ensure this. More precisely, when the distribution $p_\alpha \equiv \frac{1}{Q\|A\|}|\rho_{jk}||A_{kj}|$ is approximately unimodal and spread over many different values, one expects $a(\epsilon) \sim 1$ and $\delta(\epsilon) \ll 1$. In the setting of a system interacting with a thermal bath, this implies equilibration time scales that do not scale as the size of the bath grows, as Theorem 4.10 shows.

Whether the above holds or not ultimately boils down to the distribution of energy gaps and to the values of the off diagonal matrix elements of the observable and initial state in the energy basis. For large systems the distribution of energy levels tend to grow exponentially with energy in the region of finite temperature. It is easy to check that if one assumes a density of states $\nu(E) \propto e^{\beta E}$, the corresponding density of gaps scales like $\mu\left(|G|\right) \propto e^{-\beta|G|}$, with an exponential decrease.

This implies that, in order to have a resulting distribution that is characterised by one peak, it is sufficient to have matrix elements of A and of the initial state ρ_0 that grow sub-exponentially as a function of the energy gaps, which does not seem like a particularly strong assumption.

The remaining question is whether physically relevant cases will in general be of this form (satisfying the approximately unimodal condition and therefore "fast equilibrating") or of the other (violating the condition and therefore "slow equilibrating").

It is worthwhile comparing the conditions given here, with the assumptions made in Chapter 2 in order to prove equilibration of closed quantum systems. As we saw, equilibration can be proven by assuming that the effective dimension $d_{\text{eff}} = \frac{1}{\sum_j \rho_{jj}^2}$ (for non-degenerate spectrum for simplicity) is large, and that the Hamiltonian does not have too many degenerate energy gaps. Notice that, although we do not make these assumptions explicitly, both of them are in some sense implicit. On the one hand, a high effective dimension is related to having many energy levels populated in the system, which is necessary in order to have a distribution p_α that is spread over many different values. On the other hand, the presence of a very degenerate energy gap results in a distribution p_α such that $\delta(\epsilon) \ll 1$ does not hold, as the simple example after Theorem 4.10 illustrates.

The Eigenstate Thermalization Hypothesis, introduced by Deutsch and Srednicki as a sufficient condition for thermalization [39, 40], has motivated extensive work on the distri-

bution of diagonal matrix elements of observables [41, 88–94]. However, much less work dealing with the distribution of the off diagonal matrix elements is available, some examples being [95–98]. The findings in this chapter emphasize the importance of the off diagonal matrix elements of observable and initial state to the study of the equilibration time scales in closed quantum systems. The recent papers [96, 97] show, in certain models, gaussian distribution of these matrix elements for local observables, which supports our claim that a unimodal distribution of p_α is to be expected in many situations. Moreover, [98] numerically verifies some our predictions in an experimentally realizable quantum dot set-up.

We see our results as a step forward into a first principles proof of the equilibration of quantum systems within realistic times, for physically relevant models. It would be interesting to study whether the general conditions needed on the distribution p_α can be proven to hold for certain classes of physical systems. Moreover, we have focused mainly on the equilibration of a small system with respect to a pre-equilibrated bath, but many open questions remain regarding general equilibration timescales. One direction of particular interest is an equilibration timescale for the bath itself, and what aspects are necessary for it to play its usual thermodynamic role. We hope that the tools developed will aid in further study along these lines and help shed further light into this important topic.

Chapter 5

Non-thermal channels as a thermodynamical resource

We start this chapter by reviewing general results of work extraction from systems in non-thermal states, in a classical thermodynamics framework in Section 5.1 and in a quantum thermodynamics framework in Section 5.2. In introducing this topic for quantum mechanical systems, we distinguish between how much work can be extracted from a single system in a single instance (the single-shot case), versus the asymptotic work that can be extracted on average after many repetitions of a work extraction protocol. These sections then serve as background for Section 5.3, where we adopt the perspective of taking non-thermal channels as a resource from which work can be extracted. Given a number of non-thermal channels we find that, in the asymptotic case of many copies of the channels, the maximum extractable work is an additive function of the channels considered. We then apply this result to the case of Gaussian channels, and end up with the particular study of a channel defined by the non-unitary evolution assumed in the Ghirardi-Rimini-Weber collapse model.

5.1 Work extraction in classical thermodynamics

Assume that, in the classical thermodynamics framework, we have some target system $\mathcal{S}$ from which we wish to extract work. Experimental observation led to noticing that there is a ubiquitous existence of systems in thermal states around us. Hence, we also assume that this work extraction process can be done with free access to some *thermal bath* at a temperature T, which is assumed to be big compared to $\mathcal{S}$, so that in the whole process its state does not

change, and in particular its temperature T remains constant. The *free energy* is a central quantity behind this problem, defined as follows.

Definition 5.1 (Classical free energy)**.** *For a system with energy U and thermodynamical entropy S the free energy with respect to a bath at temperature T is*

$$F \equiv U - K_B T S, \tag{5.1}$$

where K_B is Boltzmann's constant [1]*.*

Then, the second law of thermodynamics implies that the work W that can be extracted from the system satisfies

$$W \leq -\left(F_f - F_i\right), \tag{5.2}$$

where F_f and F_i are the final and initial free energies of the target system $\mathcal{S}$, respectively, with the equality attained for quasistatic, reversible, processes [1]. Since the free energy is minimized for thermal states, the maximum work is attained when the system's final state is thermal.

5.2 Non-thermal states as thermodynamical a resource

We now address the analogous problem in quantum mechanics: given a target system $\mathcal{S}$ in an initial state ρ, how much work can we extract? Based on the results we just saw for the classical case, one might expect that as long as ρ is non-thermal some amount of work could be extracted. However, as we will see below, this is not as straightforward as it looks.

A device that can be used to store the work extracted will be referred to as the *battery*. We will take a minimalist stance on the notion of quantum work extraction, and define it as the process of exciting some two level system with Hamiltonian $H = E\left|1\right\rangle\left\langle 1\right|$ from its ground state $\left|0\right\rangle$ to the excited state $\left|1\right\rangle$. This system (or more generally, a collection of such systems) used to store the energy constitutes our battery. This is the standpoint taken in [18], but it is worth mentioning that alternative approaches can be considered. For instance, in [24] work is defined as the average energy increase of some infinite dimensional

[1] Notice we are keeping Boltzmann's constant outside of the definition of the entropy.

weight constituting the battery.

It will be useful to analyze the process of extracting work from non-thermal states in terms of a resource theory, where thermal states (i.e. thermal baths) are free to use, while any state that is not thermal becomes a resource. As a matter of fact, resource theories have been useful in different topics within quantum information theory [99–102]. The idea is similar to above: considering free access to certain operations and/or states, any state and/or operation that is not in the above set can in principle be used as a resource.

In the concrete setting of a resource theory of quantum thermodynamics, we assume unlimited access to thermal states (i.e. Gibbs states of a fixed temperature T), the freedom to apply any energy conserving unitary on system plus the bath (any unitary V that commutes with the total Hamiltonian), and the possibility of discarding part of the system or bath (i.e. apply partial traces). These rules are imported from classical thermodynamics, where one assumes access to infinite baths of constant temperature and any evolution where energy is conserved.

Given a target system $\mathcal{S}$ with Hilbert space $\mathcal{H}_\mathcal{S}$ and Hamiltonian H_S, any physical operation is represented by *a quantum channel*, i.e., a completely positive trace preserving map Ω. For simplicity, we will assume that the input and output spaces of each channel are the same.

Unitary evolution is a particular instance of a quantum channel, determined by the evolution operator. However, quantum channels allow to express more general evolutions. For example, any unitary interaction of a system with an ancilla (or environment) generates a quantum channel, given by

$$\Omega(\rho) = \mathrm{Tr}_A \left[V \rho \otimes \sigma_A V^\dagger \right], \tag{5.3}$$

where σ_A is the state of the ancilla, and V is some unitary operator. In fact, it can be shown that any channel can be generated via the above procedure [103].

Rather than allowing for any possible quantum channel, in this section we restrict to the ones that correspond to interactions with thermal states, and in which energy is conserved. Hence, we define *thermal channels* as follows.

Definition 5.2 (Thermal channel)**.** *A channel Ω_T given by*

$$\Omega_T(\rho) = \mathrm{Tr}_A \left[V \rho \otimes \sigma_A V^\dagger \right] \tag{5.4}$$

is a thermal channel at temperature T if the ancilla is in a Gibbs state of temperature T, and the unitary V commutes with the total Hamiltonian $H_T = H_S \otimes \mathbb{1}_A + \mathbb{1}_S \otimes H_A$ of the target-ancilla system.

Notice that Gibbs input states τ_{th} are invariant under thermal channels: $\Omega_T(\tau_{\mathrm{th}}) = \tau_{\mathrm{th}}$.

Now the central question is, under this allowed set of operations, how much work can one extract from the state ρ?

Depending on the nature of the work extraction protocol, there are different ways to approach this topic. One very clear distinction is between work extraction out of an individual system and in one instance, versus the average work extraction out of many repetitions of the process (or, equivalently, out of many copies of the system). The first case is referred to in the literature as the *single-shot scenario*, while we will refer to the second one as the *asymptotic scenario*.

Let us start by reviewing the asymptotic scenario, where we focus on the average work that can be extracted after repeating the procedure n times.

Proposition 5.3 (Asymptotic work extraction)**.** *In the asymptotic case of many repetitions of a work extraction protocol, the maximum average extractable work from any state ρ is given by*

$$W = F(\rho) - F(\tau_{\mathrm{th}}). \tag{5.5}$$

Here F is a quantum generalization of the classical free energy.

Definition 5.4 (Quantum free energy)**.** *For a system in a state ρ the free energy with respect to a bath at temperature T is*

$$F(\rho) = U(\rho) - K_B T S(\rho), \tag{5.6}$$

where $U(\rho) = \mathrm{Tr}\left[\rho H\right]$ is the average energy, and $S(\rho) = -\mathrm{Tr}\left[\rho \ln \rho\right]$ its von Neumann entropy.

Proposition 5.3 has many alternative proofs, see [19, 22, 24].

Another related result which will prove useful refers to the work needed in order to produce some non-thermal state. Brandão et al. proves in [19] the following.

Proposition 5.5 (Asymptotic formation of non-thermal states)**.** *The average work necessary to create a state ρ, in the asymptotic case, is given by*

$$W = F(\rho) - F(\tau_{\text{th}}), \tag{5.7}$$

as long as one has access to a sub-linear amount of coherence.

For the proof the authors make use of *catalysts*, that is, auxiliary systems which can be used in the protocol as long as they are returned in the same state in the end. They find that, unless the target system we want to construct is in a state ρ diagonal in the energy basis, an extra amount of coherence sub-linear in n may be needed to rebuild it, where n is the number of copies of ρ constructed. More specifically, for each energy transition $E_s \to E_t$ in the target system Hamiltonian H_S, the protocol proposed in the proof requires a catalyst system with Hamiltonian $H^{s,t} = \sum_{k=0}^{O(m)} (E_s - E_t) k \left|k\right\rangle \left\langle k\right|$ in state $\frac{1}{\sqrt{m}} \sum_{k=0}^{m} \left|k\right\rangle$, with m sublinear in n. When taking the asymptotic case of large n, this sublinear amount becomes negligible. At the end of the protocol such 'coherent states' will be approximately rebuilt with vanishing error. See Appendix E of [19] for the details of the proof.

The situation is quite different in the single-shot scenario. In such a case, Horodecki and Oppenheim show in [18] the following.

Proposition 5.6 (Single-shot work extraction)**.** *In the single-shot case, the deterministic extractable work is given by*

$$W = F_{\min}(\rho) - F_{\min}(\tau_{\text{th}}), \tag{5.8}$$

where $F_{\min}(\rho) \equiv K_B T \sum_E h(\omega, E) e^{-\beta E}$, ω is the state ρ dephased in the energy basis, and $h(\omega, E)$ is 1 if the energy level E is populated and 0 otherwise.

The authors also consider a relaxed single-shot scenario where a small probability of error is allowed in the work extraction protocol (in this case a generalization of $F_{\min}$ arises).

Notably, Proposition 5.6 implies the existence of non-thermal states from which no work can be extracted in one single instance. For example the authors notice that, if the energy levels $|E\rangle$ are non-degenerate, no work can be extracted from the state

$$|\Psi\rangle = \sum_E \sqrt{\frac{e^{-\beta E}}{Z}} |E\rangle . \tag{5.9}$$

This is easy to see from the fact that, when dephased, the state becomes the thermal state, so $W = 0$. However, already two copies of the state $|\Psi\rangle$ allows some work to be extracted, and in the asymptotic limit of many copies the result from Proposition 5.3 is recovered.

5.3 Non-thermal channels as a thermodynamical resource

In this section we show a complementary approach to work extraction in quantum thermodynamics, by accommodating the possibility of considering non-thermal maps, or channels, as a resource. This was a result of joint work with Miguel Navascués, and has previously been published as "Non-thermal quantum channels as a thermodynamical resource", Physical Review Letters **115**, 010405 (2015) [70].

Suppose we want to build a *thermal engine*, by integrating a number of non-thermal maps $\{\Omega_j\}_{j=1}^N$ that are accessible to us, each of which acts on a system with Hamiltonian H_j. As before, thermal states and channels will be free resources, so our machine can make use of any amount of these, and we can invoke use of each of the channels $\{\Omega_j\}_{j=1}^N$, in the order we want. Furthermore, we assume access to catalysts, i.e., we can use any number of non-thermal states as long as these are returned in the end of the work extraction protocol. Under these conditions, what is the maximum amount of work that our device can extract?

5.3.1 Single-shot case

We start by restricting to thermodynamical processes which distill work deterministically, i.e., always the same amount. The corresponding *deterministic extractable work* from a single use of a channel can then be shown to behave very badly: not only is it not additive, but it can be super-activated. That is, there exist channels Ω such that no work can be distilled from a single use, but two uses of the channel can be combined to produce a non-zero amount

of deterministic work.

In order to prove this, consider the channel Ω that takes any state of a target two level system with Hamiltonian $H = E_1 |1\rangle\langle 1|$ to the state $|\psi\rangle \propto \left(|0\rangle + e^{-\beta E_1/2}|1\rangle\right)$, i.e. $\Omega(\rho) = |\psi\rangle\langle\psi|$ for all ρ. Notice that $|\psi\rangle$ is of the kind considered in eq. (5.9).

Now, any protocol that intends to extract work from a single use of Ω can be divided into these steps:

1. The system is prepared in a state $\rho_0 = \sigma_{cat} \otimes \tau_{th} \otimes |0\rangle\langle 0|_b$, which comprises catalysts, thermal states, and the battery system (in state $|0\rangle$, ready to store work).

2. We apply an energy-conserving unitary U_1 over the whole system.

3. We apply Ω (which in this case replaces a target system's state by $|\Psi\rangle$).

4. We apply a second energy-conserving unitary U_2 over the whole system.

At the end of the protocol, the battery should have evolved to $|1\rangle$.

If, rather than implementing step 3, we add the state $|\psi\rangle$ in the preparation stage, then it is trivial to find an energy-conserving unitary $\tilde{U}_2$ that at the last step would produce exactly the same amount of work. In such a case, we would have extracted work from the resource state $|\psi\rangle$.

However, as mentioned in the discussion after Proposition 5.6 on page 79, no work can be extracted from a single copy of $|\psi\rangle$, even with the use of catalysts. This implies that the deterministic distillable work of a single use of Ω is zero.

Nevertheless, with access to two uses of Ω we could prepare two copies of $|\psi\rangle$, from which a non-zero amount of work can be deterministically extracted via thermal operations [18], showing that super-activation can occur.

5.3.2 Asymptotic case

Alternatively, we can consider thermodynamical processes which generate a given amount of work with high probability. Here the figure of merit would be the maximum amount of work that can be distilled asymptotically, on average, when we have access to n uses of each channel.

In the next pages we show that the *asymptotically extractable work* from a set of non-thermal channels $\{\Omega_j\}_{j=1}^N$ is upper bounded by $\sum_{j=1}^N W(\Omega_j, H_j)$, where

$$W(\Omega, H) \equiv \max_{\rho} \Delta F(\rho, \Omega), \tag{5.10}$$

with $\Delta F(\rho, \Omega)$ denoting the free energy difference between the states $\Omega(\rho)$ and ρ, i.e.

$$\Delta F(\rho, \Omega) \equiv \mathrm{Tr}\left[(\Omega(\rho) - \rho)H\right] - K_B T \left[S(\Omega(\rho)) - S(\rho)\right]. \tag{5.11}$$

We will refer to the quantity $W(\Omega, H)$ as the *distillable work* of channel Ω. From the inequality $\Delta F(\tau_{th}, \Omega) \geq 0$, it follows that $W(\Omega, H) \geq 0$ for any Ω.

As we will see, the bound $\sum_{j=1}^N W(\Omega_j, H_j)$ can be achieved asymptotically via a simple protocol where we prepare suitable initial states σ_{cat} (the catalysts) which maximize eq. (5.10) for each channel, and then let each channel act over its corresponding maximizer. The result of this protocol is a state with free energy $F(\sigma_{cat}) + \sum_{j=1}^N W(\Omega_j, H_j)$. Given access to n uses of each channel, we can thus prepare n copies of the latter state, whose free energy can be converted to work via Proposition 5.3 on page 78. Then Proposition 5.5 on page 79 implies that part of this work, roughly $nF(\sigma_{cat})$, can be used to regenerate the catalysts up to a small error [2]. The average work extracted with this procedure, namely the total work divided by n, is thus given by $\sum_{j=1}^N W(\Omega_j, H_j)$. Note that, as discussed after Proposition 5.5, in general an extra amount of coherence, sublinear in n, may be needed to rebuild the catalysts.

In order to prove the above result, and some later ones, the next lemma will be evoked extensively.

Lemma 5.7. *Let $\sigma^{(N)}$ be an N-partite quantum state with reduced single-site states σ_i, and let $\{\Omega_j\}_{j=1}^N$ be a collection of N single-site quantum channels. Defining $\Omega \equiv \bigotimes_{j=1}^N \Omega_j$, we have that*

$$\sum_{j=1}^{N} S\left(\sigma_j\right) - S\left(\Omega_j\left(\sigma_j\right)\right) \geq S\left(\sigma^{(N)}\right) - S\left(\Omega\left(\sigma^{(N)}\right)\right). \tag{5.12}$$

Proof. The relative entropy, defined for any two states ρ_1 and ρ_2 as $S\left(\rho_1 \| \rho_2\right) \equiv \mathrm{Tr}\left[\rho_1 \left(\ln \rho_1 - \ln \rho_2\right)\right]$,

[2] Crucially, at the end of the regeneration step the free energy of the reconstructed catalysts also tends to its initial value.

satisfies the contractivity property [104], which states that for any channel Φ,

$$S\left(\Phi(\rho_1)\|\Phi(\rho_2)\right) \leq S\left(\rho_1\|\rho_2\right). \tag{5.13}$$

From the definition of the relative entropy we can write

$$\begin{aligned}
&S\left(\Omega\left(\sigma^{(N)}\right)\|\Omega\left(\sigma_1\otimes\ldots\otimes\sigma_N\right)\right)\\
&\quad= -S\left(\Omega\left(\sigma^{(N)}\right)\right) - \mathrm{Tr}\left[\Omega\left(\sigma^{(N)}\right)\ln\left(\Omega\left(\sigma_1\otimes\ldots\otimes\sigma_N\right)\right)\right]\\
&\quad= -S\left(\Omega\left(\sigma^{(N)}\right)\right) - \sum_{j=1}^{N}\mathrm{Tr}\left[\Omega\left(\sigma^{(N)}\right)\ln\left(\Omega_j\left(\sigma_j\right)\right)\right]\\
&\quad= -S\left(\Omega\left(\sigma^{(N)}\right)\right) - \sum_{j=1}^{N}\mathrm{Tr}\left[\Omega_j\left(\sigma_j\right)\ln\left(\Omega_j\left(\sigma_j\right)\right)\right]\\
&\quad= -S\left(\Omega\left(\sigma^{(N)}\right)\right) + \sum_{j=1}^{N}S\left(\Omega_j\left(\sigma_j\right)\right),
\end{aligned} \tag{5.14}$$

by using the fact that $\ln\left(\rho_1\otimes\rho_2\right) = \ln\left(\rho_1\right)\otimes\mathbb{1}_2 + \mathbb{1}_1\otimes\ln\left(\rho_2\right)$ and $\Omega = \bigotimes_{j=1}^{N}\Omega_i$ in the third line, and in the fourth line the fact that $\sigma_j = \mathrm{Tr}_{k\neq j}\left[\sigma_1\otimes\ldots\otimes\sigma_N\right]$. Similar calculation leads to

$$S\left(\sigma^{(N)}\|\sigma_1\otimes\ldots\otimes\sigma_N\right) = -S\left(\sigma^{(N)}\right) + \sum_{j=1}^{N}S\left(\sigma_j\right). \tag{5.15}$$

Combining eqs. (5.13), (5.14), and (5.15) completes the proof. □

A direct consequence of Lemma 5.7 is that $W(\Omega, H)$, as defined by eq. (5.10), has the remarkable property of being additive.

Proposition 5.8. *Let $\{\Omega_j\}_{j=1}^{N}$ be a set of quantum channels defined over quantum systems with Hamiltonians $\{H_j\}_{j=1}^{N}$, and furthermore denote $H_T \equiv \sum_{j=1}^{N}H_j\bigotimes_{j=1}^{N}\mathbb{1}_{k\neq j}$ and $\Omega \equiv \bigotimes_{j=1}^{N}\Omega_j$. Then,*

$$W(\Omega, H_T) = \sum_{j=1}^{N}W(\Omega_j, H_j). \tag{5.16}$$

Proof. By choosing a state $\rho = \bigotimes_{j=1}^{N}\rho_j$ in eq. (5.10) we trivially have that $W(\Omega, H_T) \geq \sum_{j=1}^{N}W(\Omega_j, H_j)$, since maximizing over all possible global states ρ is more general than

maximizing each ρ_j independently.

Let us then focus on the opposite inequality. By Lemma 5.7, we have that for any ρ with reduced single site states ρ_j,

$$\sum_{j=1}^{N} S(\rho_j) - S(\Omega_j(\rho_j)) \geq S(\rho) - S(\Omega(\rho)). \tag{5.17}$$

Substituting into the expression for the free energy difference, eq. (5.11), and using the fact that the energies are additive, gives

$$\begin{aligned}\sum_{j=1}^{N} \Delta F(\rho_j, \Omega_j) &= \sum_{j=1}^{N} \mathrm{Tr}\left[(\Omega_j(\rho_j) - \rho_j)H_j\right] - K_B T \left[S(\Omega(\rho_j)) - S(\rho_j)\right] \\ &\geq \mathrm{Tr}\left[(\Omega(\rho) - \rho)H_T\right] - K_B T \left[S(\Omega(\rho)) - S(\rho)\right] \\ &= \Delta F(\rho, \Omega). \end{aligned} \tag{5.18}$$

It follows that $\sum_{j=1}^{N} W(\Omega_j, H_j) \geq W(\Omega, H_T)$, and therefore that $W(\Omega, H)$ is additive. □

We are now ready to prove that $W(\Omega, H)$ quantifies the maximum (average) amount of work one can extract from channel Ω.

Proposition 5.9. *Let $\{\Omega_j\}_{j=1}^{N}$ be a set of quantum channels defined over quantum systems with Hamiltonians $\{H_j\}_{j=1}^{N}$. Suppose that we integrate n uses of all such channels in a thermal engine $\mathcal{T}_n$, that produces a net amount of work W_n with probability $1 - \epsilon_n$. Let us further assume that the probability of failure vanishes in the limit of large n, i.e., $\lim_{n\to\infty} \epsilon_n = 0$. Under these conditions, the average asymptotic work $\bar{W} \equiv \limsup_{n\to\infty} \frac{W_n}{n}$ satisfies*

$$\bar{W} \leq \sum_{j=1}^{N} W(\Omega_j, H_j). \tag{5.19}$$

As mentioned before, this bound is achievable with the use of catalysts and a sublinear amount of quantum coherence.

Proof. In any protocol for work extraction, the initial state of the system will be given by the catalysts σ_{cat}, a number of thermal states τ_{th}, and the battery in state $|0\rangle_b$. The initial state of the system is hence $\rho_0 \equiv \sigma_{cat} \otimes \tau_{th} \otimes |0\rangle\langle 0|_b$, with free energy $F(\sigma_{cat}) + F(\tau_{th})$.

Suppose that now we apply a sequence of energy-conserving unitaries. At time t, the state of the overall system is ρ_t, and we apply the channel $\Omega_{s(t)}$ over part of the whole system ($s(t)$ indicates the system on which we are applying the channel), possibly followed by some other thermal operation. Let us analyze how the free energy of ρ_t can increase in the above step. Calling H_T the Hamiltonian of the whole system, from the definition of $W(\Omega, H)$ given by eq. (5.10), and the additivity of the distillable work, we have that:

$$\Delta F(\Omega_{s(t)} \otimes \mathbb{1}, \rho_t) \leq W(\Omega_{s(t)} \otimes \mathbb{1}, H_T) = W(\Omega_{s(t)}, H_{s(t)}). \tag{5.20}$$

Now, any intermediate energy-conserving unitary in-between the use of any two of the channels $\{\Omega_j\}_{j=1}^N$ will keep the free energy of the overall system constant. Calling $\bar{\rho}$ the state of the system at the end of the protocol, we hence have that

$$F(\bar{\rho}) \leq n \sum_{j=1}^{N} W(\Omega_j, H_j) + F(\sigma_{cat}) + F(\tau_{th}). \tag{5.21}$$

From the subadditivity of the von Neumann entropy, which states that for any ρ_{AB} of two quantum systems A and B their entropies satisfy $S(\rho_{AB}) \leq S(\rho_A) + S(\rho_B)$ [75], it follows that

$$\begin{aligned} F(\bar{\rho}) &= U(\bar{\rho}) - K_B T S(\bar{\rho}) \\ &\geq U(\bar{\rho}_{cat}) + U(\bar{\rho}_{th}) + U(\bar{\rho}_b) - K_B T \left(S(\bar{\rho}_{cat}) + S(\bar{\rho}_{th}) + S(\bar{\rho}_b)\right) \\ &= F(\bar{\rho}_{cat}) + F(\bar{\rho}_{th}) + F(\bar{\rho}_b), \end{aligned} \tag{5.22}$$

where $\bar{\sigma}_{cat}, \bar{\rho}_{th}, \bar{\rho}_b$ are, respectively, the reduced density matrices of the catalyst, thermal, and battery systems.

At the end of the protocol, the catalyst must be regenerated, i.e., $\bar{\sigma}_{cat} = \sigma_{cat}$. Also, $F(\bar{\rho}_{th}) \geq F(\tau_{th})$, since the free energy is minimized for thermal states. Therefore, from eqs. (5.21) and (5.22) the free energy of the battery satisfies

$$F(\bar{\rho}_b) \leq n \sum_{j=1}^{N} W(\Omega_j, H_j). \tag{5.23}$$

This system is expected to end up in state $|1\rangle$ with probability $1-\epsilon_n$, i.e., $\bar{\rho}_b = (1-\epsilon_n)\,|1\rangle\langle 1| + \epsilon_n \bar{\sigma}$. It follows that $F(\bar{\rho}_b) \geq (1-\epsilon_n)W_n - K_B T h(\epsilon_n)$, with $h(p) = -p\ln(p) - (1-p)\ln(1-p)$. In the asymptotic limit, with $n \to \infty$, $\epsilon_n \to 0$, the average asymptotic work satisfies

$$\limsup_{n\to\infty} \frac{W_n}{n} \leq \sum_{j=1}^{N} W(\Omega_j, H_j). \tag{5.24}$$

Note that this bound also holds if the catalysts are recovered up to an error, as long as $F(\sigma_{cat}) - F(\bar{\sigma}_{cat}) \leq o(n)$.

As mentioned, this bound is asymptotically achieved by a protocol that takes catalyst states σ_{cat} maximizing $\Delta F(\rho, \Omega)$ as inputs. After applying n times the set of channels $\{\Omega_j\}_{j=1}^N$, the free energy is $nF(\sigma_{cat}) + n\sum_{j=1}^N W(\Omega_j, H_j)$, which we know can be converted into work from Proposition 5.3. Then, from Proposition 5.5 roughly $nF(\sigma_{cat})$ of this work is necessary to rebuild the catalysts (with access to a sublinear amount of coherence), leaving us with an average distillable work $\sum_{j=1}^N W(\Omega_j, H_j)$. □

This result allows to quantify the work extraction capabilities of different channels. One can check, for instance, that no work can be distilled from a dephasing channel. Meanwhile, for a two-level system with Hamiltonian $H = E\,|1\rangle\langle 1|\,,\ E > 0$, the channel that takes any state to the excited state $|1\rangle$ provides the highest distillable work.

5.3.3 Gaussian channels

For an infinite dimensional target system, in principle there may exist quantum states possessing an infinite amount of energy. If we regard such states as unphysical, we should replace the maximization in eq. (5.10) on page 82 by an optimization over all states of finite energy. The resulting quantity will hence bound the maximum amount of work generated when the overall state of the system always has a finite amount of energy, that is, over physically conceivable thermal engines.

In infinite dimensional systems Gaussian quantum channels have a special relevance: they are easy to implement in the lab, and are extensively used to model particle interactions with a macroscopic environment (for a review of Gaussian states and channels with an emphasis on their role in quantum information see [105]). They are defined as channels which, when

composed with the identity map, transform Gaussian states into Gaussian states, the latter being those states with a Gaussian Wigner function. An m-mode Gaussian state with a density matrix ρ is completely defined via its displacement vector $\vec{d}$ and covariance matrix γ, defined by

$$d_j \equiv \mathrm{Tr}\left[R_j \rho\right], \qquad \gamma_{jk} \equiv \mathrm{Tr}\left[\left\{R_j - d_j \mathbb{1}, R_k - d_k \mathbb{1}\right\}_+ \rho\right], \tag{5.25}$$

where $(R_1, R_2, ..., R_{2m}) \equiv (Q_1, P_1, ..., Q_m, P_m)$ are the optical quadratures. The action of a Gaussian channel is fully specified by its action over the displacement vector and covariance matrix, given by:

$$\vec{d} \to X\vec{d} + \vec{z}, \qquad \gamma \to X\gamma X^T + Y, \tag{5.26}$$

where $Y + i\sigma - iX^T\sigma X \geq 0$. Here σ denotes the symplectic form $\sigma = \oplus_{i=1}^{m} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$ (see [106] for definition and properties of Gaussian states and channels).

If the Hamiltonian of the system under study is a quadratic function of the optical quadratures, i.e.,

$$H = \vec{R}^T G \vec{R} + \vec{h} \cdot \vec{R}, \tag{5.27}$$

for some real symmetric matrix G and real vector $\vec{h}$, then the average energy of a state with displacement vector $\vec{d}$ and covariance matrix γ is given by

$$U = \frac{1}{2}\mathrm{Tr}\left[G\gamma\right] + \vec{d}^T G \vec{d} + \vec{h} \cdot \vec{d}. \tag{5.28}$$

States with finite energy hence correspond to states with finite first and second moments. When the quadratic Hamiltonian is such that $G > 0$, i.e. if it has no zero energy modes, Proposition 5.9 on page 84 allows to classify generic Gaussian channels according to their capacity to generate an infinite amount of work. Indeed, for $X^T G X - G \not\leq 0$, the channel's distillable work is unbounded, which can be seen by inputting a sequence of Gaussian states with constant covariance matrix but increasing displacement vector parallel to any positive eigenvector of $X^T G X - G$, with corresponding eigenvalue λ. This leads to an increase in

energy, after applying such channel once, given by

$$\Delta U = \vec{d}^T X^T G X \vec{d} - \vec{d}^T G \vec{d} + \vec{h}^T X \vec{d} - \vec{h} \cdot \vec{d} = \lambda + \vec{h}^T X \vec{d} - \vec{h} \cdot \vec{d}, \tag{5.29}$$

which is not upper bounded when one maximizes over any input state, simply because one can always take a larger λ. Since the von Neumann entropy is constant for constant covariance matrix [105](or see eq. (5.43) on page 92 below), this leads to a free energy $F(\rho, \Omega)$, and consequently distillable work, which are unbounded.

Conversely, as we show in Appendix A.4, for channels satisfying $X^T G X - G < 0$ only a finite amount of work can be distilled.

For such channels there is still the dilemma of how much work can be extracted. We now show that this problem can be greatly simplified, by proving that the maximization in eq. (5.10) on page 82 can be restricted to Gaussian states. The following result will prove useful.

Lemma 5.10. *Let ρ be an arbitrary state with finite first and second moments, and let ρ_G be the unique Gaussian state with the same first and second moments. Then, for any Gaussian channel Ω, we have that*

$$S(\rho_G) - S(\Omega(\rho_G)) \geq S(\rho) - S(\Omega(\rho)). \tag{5.30}$$

Proof. Let the action of Ω over the displacement vector and covariance matrix be given by eq. (5.26). Since von Neumann entropies remain the same after a unitary transformation, without loss of generality we will assume that ρ's displacement vector is null, and that $z = 0$ in the channel description (5.26) of Ω. Now, let U_n be the n-system "Gaussification" transformation described in [107]. Calling $\tilde{\rho}^{(n)} = U_n \rho^{\otimes n} U_n^\dagger$, we have that

$$\begin{aligned} L_n &\equiv \sum_{j=1}^{n} S\left(\tilde{\rho}_j\right) - S\left(\Omega\left(\tilde{\rho}_j\right)\right) \\ &\geq S\left(\tilde{\rho}^{(n)}\right) - S\left(\Omega^{\otimes n}\left(\tilde{\rho}^{(n)}\right)\right) \\ &= S\left(\rho^{\otimes n}\right) - S\left(\Omega^{\otimes n}(\rho^{\otimes n})\right) \\ &= n\{S\left(\rho\right) - S\left(\Omega(\rho)\right)\}, \end{aligned} \tag{5.31}$$

where the inequality is due to Lemma 5.7 on page 82, and the equality in the third line follows from using that the von Neumann entropy is invariant under global unitaries, and the fact that for any state σ,

$$\Omega^{\otimes n}(U_n \sigma U_n^\dagger) = U_n \Omega^{\otimes n}(\sigma) U_n^\dagger. \tag{5.32}$$

This identity follows from three observations:
1) any Gaussian channel with $z = 0$ is the result of applying a symplectic unitary V_S over the target system and an ancillary Gaussian state ρ_A with zero displacement vector [108];
2) n copies of ρ_A are invariant with respect to a Gaussification operation U_n^A (given that ρ_A is already a Gaussian state);
3) since U_n^A and U_n are Gaussification operations, it holds that $V_S^{\otimes n} U'_n \sigma \otimes \rho_A^{\otimes n} U_n'^\dagger \left(V_S^{\otimes n}\right)^\dagger = U'_n V_S^{\otimes n} \sigma \otimes \rho_A^{\otimes n} \left(V_S^{\otimes n}\right)^\dagger U_n'^\dagger$, where $U'_n = U_n \otimes U_n^A$ represents the Gaussification of n copies of the system target-ancilla.

Since the von Neumann entropy is continuous in trace norm with respect to collections of states with finite second moments, by [107] (see the proof of their Lemma 1), we end up with

$$\begin{aligned} \lim_{n\to\infty} \frac{L_n}{n} &= \lim_{n\to\infty} \frac{1}{n} \sum_{j=1}^{n} S(\tilde{\rho}_j) - S(\Omega(\tilde{\rho}_j)) \\ &= S(\rho_G) - S(\Omega(\rho_G)). \end{aligned} \tag{5.33}$$

The lemma hence follows from eqs. (5.31) and (5.33). □

We are now ready to prove that for Gaussian channels the distillable work is attained for Gaussian input states.

Proposition 5.11. *Consider a continuous variable quantum system of m modes, with quadratic Hamiltonian H, let Ω be a Gaussian channel mapping m modes to m modes, and denote by $\mathcal{G}$ the set of all m-mode Gaussian states. Then,*

$$W(\Omega, H) = \max_{\rho \in \mathcal{G}} \Delta F(\rho, \Omega). \tag{5.34}$$

Proof. Let ρ be an arbitrary state with finite energy (and thus finite first and second moments), and let ρ_G be the Gaussian state with the same first and second moments. Then, ρ and ρ_G have the same average energy, and since Ω is a Gaussian channel the same is true for $\Omega(\rho)$ and $\Omega(\rho_G)$. However, by Lemma 5.10, the entropic change is bigger for ρ_G, and so $\Delta F(\rho_G, \Omega) \geq \Delta F(\rho, \Omega)$. □

Since $W(\Omega, H)$ just involves an optimization over a finite set of parameters subject to positive semidefinite constraints, (in principle) it can be computed exactly for any Gaussian channel Ω.

5.3.4 The collapse engine

In order to address the measurement problem [109], and, independently, the decoherence effects that a quantum theory of gravity could impose on the wave-function [110, 111], different authors have proposed that *closed* quantum systems should evolve according to the Lindblad equation

$$\frac{d}{dt}\rho_t = -\frac{i}{\hbar}[H, \rho_t] - \frac{\Lambda}{4}[X, [X, \rho_t]], \tag{5.35}$$

where X is the position operator for the particle considered.

The effect of the non-unitary term is a suppression of coherences in the position basis, effectively destroying quantum superpositions. The value of the constant Λ, which can be interpreted as the rate at which this localization process occurs, depends on the particular theory invoked to justify eq. (5.35). In the Ghirardi-Rimini-Weber (GRW) theory [109], the localization process is postulated to solve the measurement problem in quantum mechanics. To achieve this goal and avoid contradictions with past experimental results, Λ must be roughly between $10^{-2}s^{-1}m^{-2}$ and $10^{6}s^{-1}m^{-2}$, according to latest estimations [112].

Note that the above evolution is non-thermal. Hence, it could be used in principle to extract work from nothingness by means of a suitable thermal engine. We will call such a hypothetical device a *collapse engine*.

To connect this to our previous setting, notice that the evolution equation (5.35) defines

a quantum channel

$$\Omega_{\delta t}(\rho_t) = \rho_{t+\delta t}, \tag{5.36}$$

with ρ_t the solution of eq. (5.35) for the initial state ρ_0.

As a case study we focus on a particle of mass m subject to a harmonic potential of frequency ω,

$$H = \frac{m\omega^2}{2}X^2 + \frac{1}{2m}P^2. \tag{5.37}$$

Furthermore, we assume that, despite the GRW dynamics, the bath's temperature T is constant. A physical justification for this last assumption is that the temperature-increasing GRW dynamics is countered by radiation from the bath into outer space. Hence, as a function of time, the temperature will converge to a stationary value $T = T_{eq}$ above the temperature of the cosmic microwave background (CMB) [3].

In these conditions, we wish to find the maximum amount of work that a collapse engine could extract if it had access to the evolution equation (5.35) for a finite amount of time t. From Proposition 5.9 on page 84, this amounts to computing $\lim_{\delta t\to 0} \frac{t}{\delta t} W(\Omega_{\delta t}, H)$.

From the GRW evolution, and the canonical commutation relations for X and P, it is easy to check that,

$$\frac{d}{dt}\mathrm{Tr}\big(\rho_t X^2\big) = \frac{1}{m}\mathrm{Tr}\Big(\rho_t(XP+PX)\Big) \tag{5.38}$$

$$\frac{d}{dt}\mathrm{Tr}\big(\rho_t P^2\big) = -m\omega^2\mathrm{Tr}\Big(\rho_t(XP+PX)\Big) + \frac{\hbar^2}{2}\Lambda, \tag{5.39}$$

which leads to an the energy increase of any input state after the use of the channel given by

$$\Delta U = \frac{\hbar^2\Lambda}{4m}\delta t. \tag{5.40}$$

Since the GRW evolution increases the entropy of any state, as shown by Ghirardi, Rimini,

[3] If we model the bath as a grey body, then it radiates energy at a rate of $\sigma(T^4 - T_c^4)$, where T_c is the temperature of the CMB and σ is a constant that depends on how well isolated the bath is. The power transferred to the bath by the GRW dynamics is, on the other hand, independent of T and proportional to Λ. It follows that the bath will reach a stationary temperature T_{eq} whose exact value will depend on both σ and Λ.

and Weber in their original paper, we obtain

$$W(\Omega_{\delta t}, H) \leq \Delta U. \tag{5.41}$$

In order to estimate the entropy increase, notice that, since the evolution dictated by eq. (5.35) takes Gaussian states into Gaussian states [113], the channel $\Omega_{\delta t}$ is Gaussian. Hence, from Proposition 5.11, it is enough to just consider Gaussian states. A useful simplification for calculating the entropy of such states comes from Williamson's theorem, which allows to transform any covariance matrix representing a Gaussian state into a matrix proportional to the identity by a symplectic transformation [105]. Therefore, the covariance matrix γ becomes, in some new set of coordinates,

$$\gamma_{aux} = (2N+1)\mathbb{1}, \tag{5.42}$$

where N is positive. The covariance matrix γ_{aux} represents a thermal state, and for such states the entropy is given by

$$S = (N+1)\log(N+1) - N\log(N), \tag{5.43}$$

$$\det(\gamma_{aux}) = (2N+1)^2. \tag{5.44}$$

Since neither the determinant of the covariance matrix nor the entropy of the corresponding state are affected by the symplectic transformation, the above expressions also determine the entropy of our system, with $\det(\gamma) = (2N+1)^2$.

Straightforward calculations show

$$\frac{d}{dt}\operatorname{Tr}\left[\rho_t XP\right] = \frac{1}{m}\operatorname{Tr}\left[\rho_t P^2\right] - m\omega^2 \operatorname{Tr}\left[\rho_t X^2\right], \tag{5.45}$$

which, by using the expression for the covariance matrix (in SI units)

$$\gamma = \begin{pmatrix} \frac{2m\omega}{\hbar}\operatorname{Tr}\left[\rho X^2\right] & \frac{1}{\hbar}\operatorname{Tr}\left[\rho\left(XP+PX\right)\right] \\ \frac{1}{\hbar}\operatorname{Tr}\left[\rho\left(XP+PX\right)\right] & \frac{2}{m\hbar\omega}\operatorname{Tr}\left[\rho P^2\right] \end{pmatrix}, \tag{5.46}$$

and eqs. (5.38) and (5.39), leads to

$$\begin{aligned}\frac{d}{dt}N &= \frac{1}{4(2N+1)}\frac{d}{dt}\det(\gamma)\\ &= \frac{4}{\hbar^2(2N+1)}\frac{d}{dt}\Big(4\,\mathrm{Tr}\left[\rho_t X^2\right]\mathrm{Tr}\left[\rho_t P^2\right]-\left(\mathrm{Tr}\left[\rho_t\left(XP+PX\right)\right]\right)^2\Big)\\ &= \frac{\Lambda}{2(2N+1)}\,\mathrm{Tr}\left[\rho_t X^2\right].\end{aligned} \tag{5.47}$$

Thus, we obtain that the entropy change of the state can be made as small as desired by imputing a state with small $\mathrm{Tr}\left[\rho_t X^2\right]$, and so the bound in eq. (5.41) can be saturated, leading to $W(\Omega_{\delta t}, H) = \Delta U$.

Consequently, the maximum power at which a collapse engine could in principle operate is given by

$$\frac{dW}{dt} = \frac{\hbar^2\Lambda}{4m}. \tag{5.48}$$

Using the upper range estimation $\Lambda \sim 10^6 s^{-1}m^{-2}$, we have that a collapse engine powered by a single electron would produce $\frac{dW}{dt} \sim 10^{-32}$ *watt*. Assuming total control over the electrons of a macroscopic sample, one would need a kiloton of Hydrogen to power a 40 *watt* light bulb.

5.4 Discussion

In this chapter we investigated the possibility of using non-thermal channels as a resource. While non-thermal states have been widely regarded as a resource (see discussion in Section 5.2), and the quantum thermodynamics arena has not been restricted to thermal operations [114–117], we have focused on their potential as a resource, in particular for work extraction.

We addressed the problem of determining the maximum amount of work that can be extracted from these operational -as opposed to state- resources. We found that the single-shot and asymptotic scenarios widely differ. On the one hand, there exist channels from which no work can be extracted in a single instance, while access to two or more copies of the channel allow work extraction. Meanwhile, we proved that the solution to this problem in the asymptotic limit of access to many copies of a set of channels is given by a single-

letter formula that quantifies the amount of distillable work that a channel can, in principle, generate when supplemented with thermal operations and catalyst input states.

Moreover, we found how to determine the asymptotic distillable work for bosonic channels, and computed it exactly for the case of the GRW collapse dynamics, hence determining the maximum power which a hypothetical collapse engine could provide for free. Note that, in performing this calculation, we have assumed that the non-unitary GRW dynamics do not affect the results in Section 5.2 on quantum work extraction from non-thermal states (i.e. Propositions 5.3 and 5.5). Essentially, we have overlooked the fact that a fundamental modification to unitary evolution could, in principle, have further implications on the rules of thermodynamics than the ones implied by Section 5.3.4.

Note that we have only studied operational resources regarding their capacity to generate work. An interesting topic for future research is to extend these results to more general settings, with other quantities apart from thermodynamical work in mind.

Appendix A

Calculations

A.1 Typical measurements

A.1.1 Proof of Theorem 3.8

Given the projector

$$\Pi_U = \rho_0 + P_U, \qquad P_U = UPU^\dagger, \tag{A.1}$$

where ρ_0 is the initial (pure) state, U is a partial unitary with $UU^\dagger = U^\dagger U = \mathbb{1}_{\mathcal{H}'}$, P is any rank-$(K-1)$ projector with support on $\mathcal{H}'$, we want to prove

$$\langle \mathcal{D}_{\Pi_U}(\rho_t, \omega)\rangle_U \leq \mathcal{D}_{\rho_0}(\rho_t, \omega) + \frac{1}{2\sqrt{d-1}}. \tag{A.2}$$

Firstly, we have

$$\begin{aligned}
\langle \mathcal{D}_{\Pi_U}(\rho_t, \omega)\rangle_U &= \langle |\mathrm{Tr}\left[\Pi_U(\rho_t - \omega)\right]|\rangle_U \\
&\leq \sqrt{\left\langle \Big(\mathrm{Tr}\left[\Pi_U(\rho_t - \omega)\right] \Big)^2 \right\rangle_U} \\
&= \sqrt{\mathrm{Tr}\left[\langle \Pi_U \otimes \Pi_U\rangle_U (\rho_t - \omega)^{\otimes 2} \right]}.
\end{aligned} \tag{A.3}$$

Using lemma 3.5 on page 41, and the expressions for α and β that follow it, one can see that

$$\begin{aligned}\langle \Pi_U \otimes \Pi_U \rangle_U &= \langle \rho_0 \otimes \rho_0 + \rho_0 \otimes P_U + P_U \otimes \rho_0 + P_U \otimes P_U \rangle_U \\ &= \rho_0 \otimes \rho_0 + \rho_0 \otimes \langle P_U \rangle_U + \langle P_U \rangle_U \otimes \rho_0 + \langle P_U \otimes P_U \rangle_U \\ &= \rho_0 \otimes \rho_0 + \frac{K'}{d'} \rho_0 \otimes \mathbb{1}' + \frac{K'}{d'} \mathbb{1}' \otimes \rho_0 + \frac{K'(K'+1)}{d'(d'+1)} \Pi'_S + \frac{K'(K'-1)}{d'(d'-1)} \Pi'_A,\end{aligned} \tag{A.4}$$

where $\mathbb{1}' = \mathbb{1} - \rho_0$, $\Pi'_S = \mathbb{1}'^{\otimes 2} \Pi_S \mathbb{1}'^{\otimes 2}$ and $\Pi'_A = \mathbb{1}'^{\otimes 2} \Pi_A \mathbb{1}'^{\otimes 2}$.

Therefore,

$$\begin{aligned}\left\langle \Big(\operatorname{Tr}\left[\Pi_U(\rho_t - \omega)\right] \Big)^2 \right\rangle_U &= \operatorname{Tr}\left[\langle \Pi_U \otimes \Pi_U \rangle_U \, (\rho_t - \omega)^{\otimes 2} \right] \\ &= f(t)^2 - 2f(t)^2 \frac{K'}{d'} + \frac{K'(K'+1)}{d'(d'+1)} \operatorname{Tr}\left[\Pi_S A(t)\right] \\ &\quad + \frac{K'(K'-1)}{d'(d'-1)} \operatorname{Tr}\left[\Pi_A A(t)\right],\end{aligned} \tag{A.5}$$

where $A(t) = \left[(\mathbb{1} - \rho_0)(\rho_t - \omega)(\mathbb{1} - \rho_0)\right]^{\otimes 2}$, and $f(t) \equiv \mathcal{D}_{\rho_0}(\rho_t, \omega) = \operatorname{Tr}\left[\rho_0(\rho_t - \omega)\right]$.

Moreover,

$$\begin{aligned}\operatorname{Tr}\left[\Pi_S A(t)\right] &= \operatorname{Tr}\left[\frac{\mathbb{1}^{\otimes 2} + \$}{2} \left[(\mathbb{1} - \rho_0)(\rho_t - \omega)(\mathbb{1} - \rho_0)\right]^{\otimes 2} \right] \\ &= \frac{1}{2} \operatorname{Tr}\left[(\mathbb{1} - \rho_0)(\rho_t - \omega)(\mathbb{1} - \rho_0)(\rho_t - \omega)\right] + \frac{1}{2} \Big(\operatorname{Tr}\left[\rho_t - \omega - \rho_0(\rho_t - \omega)\right] \Big)^2 \\ &\leq \frac{1}{2} \left(1 - \frac{1}{d_{\text{eff}}}\right) + \frac{1}{2} \left(f(t)\right)^2,\end{aligned} \tag{A.6}$$

where the last line is due to $\operatorname{Tr}\left[\Pi X \Pi X\right] \leq \operatorname{Tr}\left[X^2\right]$ for a projector Π (in this case, $\mathbb{1} - \rho_0$), which follows from the Cauchy-Schwarz inequality $\operatorname{Tr}\left[\Pi X \Pi X\right] \leq \sqrt{\operatorname{Tr}\left[X^2\right] \operatorname{Tr}\left[\Pi X \Pi X\right]}$.

Finally, using that

$$\begin{aligned}\operatorname{Tr}\left[\Pi_A A(t)\right] &= \operatorname{Tr}\left[\frac{\mathbb{1}^{\otimes 2} - \$}{2} \left[(\mathbb{1} - \rho_0)(\rho_t - \omega)\right]^{\otimes 2} \right] \\ &\leq \frac{1}{2} \left(f(t)^2 - 1 + \frac{1}{d_{\text{eff}}} \right),\end{aligned} \tag{A.7}$$

we have

$$\begin{aligned}\left\langle \Big(\operatorname{Tr}\left[\Pi_U(\rho_t-\omega)\right]\Big)^2 \right\rangle_U &\leq f(t)^2\left(1+\frac{1}{2}\frac{K'(K'+1)}{d'(d'+1)}+\frac{1}{2}\frac{K'(K'-1)}{d'(d'-1)}-2\frac{K'}{d'}\right)\\ &\quad+\frac{1}{2}\left(1-\frac{1}{d_{\text{eff}}}\right)\left[\frac{K'(K'+1)}{d'(d'+1)}-\frac{K'(K'-1)}{d'(d'-1)}\right]\\ &= f(t)^2\left(1-2\frac{K'}{d'}+\frac{K'}{d'}\frac{K'd'-1}{d'^2-1}\right)+\left(1-\frac{1}{d_{\text{eff}}}\right)\frac{K'}{d'}\frac{d'-K'}{d'^2-1}\\ &\leq f(t)^2+\frac{1}{4d'}\\ &= \mathcal{D}^2_{\rho_0}(\rho_t,\omega)+\frac{1}{4(d-1)}. \end{aligned} \tag{A.8}$$

The previous to last line can be derived from the fact that the first parentheses in the penultimate equation is maximized by $K'=0$, and the second term is maximized by $K'=d'/2$, along with $d_{\text{eff}}\leq d$ and $\frac{d'^2}{(d'-1)(d'+1)^2}\leq\frac{1}{d'}$. Combining this with eq. (A.3) finishes the proof.

A.1.2 Proof of Corollary 3.10

Denoting by K_j the rank of P_j, we have that

$$\sum_j K_j = d' \tag{A.9}$$

and

$$\begin{aligned}\left\langle \mathcal{D}_{\mathcal{M}_U^{\rho_0}}(\rho_t,\omega)\right\rangle_U &= \frac{1}{2}\left\langle \mathcal{D}_{\rho_0+P_{1U}}(\rho_t,\omega)\right\rangle_U+\frac{1}{2}\sum_{j=2}^N\left\langle \mathcal{D}_{P_{jU}}(\rho_t,\omega)\right\rangle_U\\ &\leq \frac{1}{2}\sqrt{\left\langle \mathcal{D}_{\rho_0+P_{1U}}(\rho_t,\omega)^2\right\rangle_U}+\frac{1}{2}\sum_{j=2}^N\sqrt{\left\langle \mathcal{D}_{P_{jU}}(\rho_t,\omega)^2\right\rangle_U}. \end{aligned} \tag{A.10}$$

Following the proof in Appendix A.1.1 above, and using the fact that $1-\frac{1}{d_{\text{eff}}}\leq 1-\frac{1}{d}=\frac{d'}{d'+1}$, leads to

$$\left\langle \mathcal{D}_{P_{jU}}(\rho_t,\omega)^2\right\rangle_U \leq f(t)^2\frac{K_j}{d'}\frac{K_jd'-1}{d'^2-1}+\frac{K_j}{d'+1}\frac{d'-K_j}{d'^2-1} \tag{A.11}$$

and

$$\begin{aligned}\left\langle \mathcal{D}_{\rho_0+P_{1U}}(\rho_t,\omega)^2\right\rangle_U &\leq f(t)^2\left(1-2\frac{K_1}{d'}+\frac{K_1}{d'}\frac{K_1d'-1}{d'^2-1}\right)+\frac{K_1}{d'+1}\frac{d'-K_1}{d'^2-1}\\ &\leq f(t)^2\left(1+\frac{K_1}{d'}\frac{K_1d'-1}{d'^2-1}\right)+\frac{K_1}{d'+1}\frac{d'-K_1}{d'^2-1}\\ &= f(t)^2+\left\langle \mathcal{D}_{P_{1U}}(\rho_t,\omega)^2\right\rangle_U. \end{aligned} \tag{A.12}$$

By using the fact that $\sqrt{a+b}\leq\sqrt{a}+\sqrt{b}$ for $a,b\geq 0$, this leads to

$$\left\langle \mathcal{D}_{\mathcal{M}_U^{\rho_0}}(\rho_t,\omega)\right\rangle_U \leq \frac{1}{2}\left|f(t)\right|+\frac{1}{2}\sum_{j=1}^{N}\sqrt{\left\langle \mathcal{D}_{P_{jU}}(\rho_t,\omega)^2\right\rangle_U}. \tag{A.13}$$

Through the method of Lagrange multipliers it is easy to see that the sum in eq. (A.13), expressed in terms of the K_j's through eq. (A.11) and constrained by eq. (A.9), is maximized by taking all P_j to be of equal rank. This rank must then be $K_j = d'/N$. Substituting that into eq. (A.11), and using the inequalities $\frac{d'^2-N}{d'^2-1}<1$, $1-1/N<1$ and $d'^3\leq(d'+1)^2(d'-1)$,

$$\begin{aligned}\left\langle \mathcal{D}_{\mathcal{M}_U^{\rho_0}}(\rho_t,\omega)\right\rangle_U &\leq \frac{1}{2}\left|f(t)\right|+\frac{1}{2}N\sqrt{\frac{f(t)^2}{N^2}\frac{d'^2-N}{d'^2-1}+\frac{d'/N}{d'+1}\frac{d'\left(1-\frac{1}{N}\right)}{d'^2-1}}.\\ &\leq \frac{1}{2}\left|f(t)\right|+\frac{1}{2}\sqrt{f(t)^2+\frac{Nd'^2}{(d'+1)^2(d'-1)}}.\\ &\leq \left|f(t)\right|+\frac{1}{2}\sqrt{\frac{N}{d'}}. \end{aligned} \tag{A.14}$$

A.2 Truncation of the Hilbert space: Theorem 4.10

Let us start by writing the initial (untruncated) state in the basis $|j\rangle$ of eigenvectors of the full Hamiltonian H as

$$\rho_0 = \sum_{jk} \rho_{jk} |j\rangle \langle k| . \tag{A.15}$$

The truncated state is then

$$\Pi\rho_0\Pi = \sum_{jk\in J} \rho_{jk} |j\rangle \langle k| , \tag{A.16}$$

where Π projects to the truncated Hilbert space $\mathcal{H}_{H_S+H_B+H_I}^{E_B,\Delta+2\|H_S\|+\eta}$, and J is the set of eigenvalues of $H_S + H_B + H_I$ restricted to such space.

It will be useful to expand the Hilbert space to two include two new energy eigenvectors $|j_{\min}\rangle$ and $|j_{\max}\rangle$, with corresponding energies $E_{\min}$ and $E_{\max}$ respectively, such that the new Hamiltonian is

$$\overline{H} \equiv H + E_{\min} |j_{\min}\rangle \langle j_{\min}| + E_{\max} |j_{\max}\rangle \langle j_{\max}| . \tag{A.17}$$

Next, we define a new density matrix on the enlarged space by

$$\begin{aligned}\overline{\rho}_0 \equiv \zeta \Bigg(\Pi\rho_0\Pi + \frac{|x|}{2} |j_{\min}\rangle \langle j_{\min}| + \frac{x}{2} |j_{\min}\rangle \langle j_{\max}| \\ + \frac{x}{2} |j_{\max}\rangle \langle j_{\min}| + \frac{|x|}{2} |j_{\max}\rangle \langle j_{\max}| \Bigg) ,\end{aligned} \tag{A.18}$$

where x is a real constant, and ζ is an appropriate normalization constant to ensure that $\mathrm{Tr}\,[\overline{\rho}_0] = 1$. The above definition ensures that $\overline{\rho}_0$ remains a positive operator. Note also that Π is orthogonal to $|j_{\min}\rangle$ and $|j_{\max}\rangle$, since the truncation we perform is in the original Hilbert space.

Moreover, we define an observable $\overline{A}$ in a similar way, as

$$\begin{aligned}\overline{A} \equiv \frac{1}{\zeta} \Bigg(\Pi A\Pi + \frac{\|A\|}{2} |j_{\min}\rangle \langle j_{\min}| + \frac{\|A\|}{2} |j_{\min}\rangle \langle j_{\max}| \\ + \frac{\|A\|}{2} |j_{\max}\rangle \langle j_{\min}| + \frac{\|A\|}{2} |j_{\max}\rangle \langle j_{\max}| \Bigg) .\end{aligned} \tag{A.19}$$

In the derivation of Theorem 4.3, the commutators which appear in the denominator of equation (4.13) came from the standard deviation of the distribution p_α, as explained in Section 4.2. We intend to use $\overline{\rho}_0$ and $\overline{A}$ as the initial state and observable for our calculation, while proving that x can be taken such that the following conditions are fulfilled:

(i) $\quad \overline{\sigma}_G^2 \geq \frac{1}{\overline{Q}\|\overline{A}\|}\Big|\mathrm{Tr}\Big(\big[\,[\rho_0, H]\,, H\big]\,A\Big)\Big|$,

(ii) $\{\overline{\rho}_0, \overline{A}, \overline{H}\}$ lead to approximately the same physics as $\{\rho_0, A, H\}$,

where $\overline{Q}$ and $\overline{\sigma}_G$ are, respectively, the normalization factor and standard deviation of the distribution $\overline{p}_\alpha$ corresponding to $\overline{\rho}_0$ and $\overline{A}$.

Point (i) will lead to a result in Theorem 4.10 on page 67 with commutators involving the original triple $\{\rho_0, A, H\}$, as desired, while (ii) allows to use these redefined state, observable and Hamiltonian instead of the original ones.

A.2.1 Going from $\{\overline{\rho}_0, \overline{A}, \overline{H}\}$ to commutators involving $\{\rho_0, A, H\}$

Let us revisit eq. (4.15) on page 55, this time with the state $\overline{\rho}_0$ and the observable $\overline{A}$. We can see

$$\begin{aligned}
\overline{\sigma}_G^2 &= \sum_\alpha \overline{p_\alpha} G_\alpha^2 = \frac{1}{\overline{Q}\|\overline{A}\|} \sum_{j\neq k} |\overline{\rho}_{jk}||\overline{A}_{kj}|(E_j - E_k)^2 \\
&= \frac{1}{\overline{Q}\|\overline{A}\|} \left(\sum_{jk\in J} |\rho_{jk}||A_{kj}|(E_j - E_k)^2 + 2\frac{|x|}{2}\frac{\|A\|}{2} G_{\max}^2 \right) \\
&\geq \frac{1}{\overline{Q}\|\overline{A}\|} \left(\Big| \sum_{jk\in J} \rho_{jk} A_{kj} (E_j - E_k)^2 \Big| + \frac{x\|A\|}{2} G_{\max}^2 \right), \qquad \text{(A.20)}
\end{aligned}$$

where we defined the maximum energy gap $G_{\max} \equiv E_{\max} - E_{\min}$.

We now *impose* that x is such that

$$\begin{aligned}
&\frac{1}{\overline{Q}\|\overline{A}\|}\left(\Big|\sum_{jk\in J}\rho_{jk}A_{kj}(E_j-E_k)^2\Big|+\frac{x\|A\|}{2}G_{\max}^2\right)\\
&\quad\equiv\frac{1}{\overline{Q}\|\overline{A}\|}\Big|\sum_{jk}\rho_{jk}A_{kj}(E_j-E_k)^2\Big|\\
&\quad=\frac{1}{\overline{Q}\|\overline{A}\|}\Big|\mathrm{Tr}\Big(\big[\,[\rho_0,H]\,,H\big]A\Big)\Big|,
\end{aligned}\tag{A.21}$$

which together with eq. (A.20) already gives condition (i).

From the equation above we obtain

$$\begin{aligned}
x\frac{\|A\|G_{\max}^2}{2}&=\Big|\sum_{jk}\rho_{jk}A_{kj}(E_j-E_k)^2\Big|-\Big|\sum_{jk\in J}\rho_{jk}A_{kj}(E_j-E_k)^2\Big|\\
&\le\Big|\sum_{jk}\rho_{jk}A_{kj}(E_j-E_k)^2-\sum_{jk\in J}\rho_{jk}A_{kj}(E_j-E_k)^2\Big|\\
&=\Big|\mathrm{Tr}\Big(\big[\,[\rho_0-\Pi\rho_0\Pi,H]\,,H\big]A\Big)\Big|\\
&=\Big|\mathrm{Tr}\Big(\big[\,[\rho_0-\Pi\rho_0\Pi,H']\,,H'\big]A\Big)\Big|,
\end{aligned}\tag{A.22}$$

where in the last line we define the auxiliary Hamiltonian $H'\equiv H-\frac{E_{\max}+E_{\min}}{2}\mathbb{1}$, shifted so that its spectrum is centered around 0. By noting that $\|H'\|=\|H\|-\frac{E_{\max}+E_{\min}}{2}=\frac{E_{\max}-E_{\min}}{2}=\frac{G_{\max}}{2}$, expanding the four terms in the above commutators, using that for any two operators O and P one has $\mathrm{Tr}\,[OP]\le\|O\|\|P\|_1$ from Holder's inequality, and Proposition 4.6 on page 61 , we end up with

$$\begin{aligned}
x\ &\le\frac{2}{\|A\|G_{\max}^2}4\|\rho_0-\Pi\rho_0\Pi\|_1\|A\|\|H'\|^2\\
&=2\,\|\rho_0-\Pi\rho_0\Pi\|_1\\
&\le\frac{4}{K}.
\end{aligned}\tag{A.23}$$

Similarly, we can show that $-x\le\frac{4}{K}$, and hence that

$$|x|\le\frac{4}{K}.\tag{A.24}$$

A.2.2 $\{\overline{\rho}_0, \overline{A}, \overline{H}\}$ give approximately the same physics as $\{\rho_0, A, H\}$

We now check that condition (ii) is also satisfied. Note that

$$\begin{aligned}
\left| \operatorname{Tr}\left[\rho_0 A\right] - \operatorname{Tr}\left[\overline{\rho}_0 \overline{A}\right] \right| &\leq \left| \operatorname{Tr}\left[\rho_0 A\right] - \operatorname{Tr}\left[\Pi\rho_0\Pi A\right] \right| + \left| \operatorname{Tr}\left[\Pi\rho_0\Pi A\right] - \operatorname{Tr}\left[\overline{\rho}_0 \overline{A}\right] \right| \\
&= \left| \operatorname{Tr}\left[\rho_0 A\right] - \operatorname{Tr}\left[\Pi\rho_0\Pi A\right] \right| + \left| \frac{x\|A\|}{2} + \frac{|x|\|A\|}{2} \right| \\
&\leq \|\rho_0 - \Pi\rho_0\Pi\|_1 \|A\| + |x|\|A\| \\
&\leq \frac{2\|A\|}{K} + \frac{4\|A\|}{K}, \qquad \text{(A.25)}
\end{aligned}$$

by using in the third line that $\operatorname{Tr}\left[\overline{\rho}_0 \overline{A}\right] = \operatorname{Tr}\left[A\Pi\rho_0\Pi\right] + 2\frac{x\|A\|}{4} + 2\frac{|x|\|A\|}{4}$ (which comes from the definition of $\overline{A}$ and $\overline{\rho}_0$), and the fact that Π is orthogonal to $|j_{\min}\rangle$ and $|j_{\max}\rangle$.

The above equation justifies the approach of defining auxiliary state and observable, since we proved that these mimic the original state and observable in the predictions.

The result can be translated into the weak-distinguishability between ρ_t and ω. By the triangle inequality, a similar calculation as above, and the fact that the trace distance is invariant under unitary evolution, we see

$$\begin{aligned}
\left|\operatorname{Tr}\left[\rho_t A\right] - \operatorname{Tr}\left[\omega A\right]\right|^2 &\leq \left|\operatorname{Tr}\left[\rho_t A\right] - \operatorname{Tr}\left[\overline{\rho}_t \overline{A}\right]\right|^2 + \left|\operatorname{Tr}\left[\overline{\rho}_t \overline{A}\right] - \operatorname{Tr}\left[\overline{\omega}\overline{A}\right]\right|^2 \\
&\quad + \left|\operatorname{Tr}\left[\overline{\omega}\overline{A}\right] - \operatorname{Tr}\left[\omega A\right]\right|^2 \\
&\leq \left|\operatorname{Tr}\left[\overline{\rho}_t \overline{A}\right] - \operatorname{Tr}\left[\overline{\omega}\overline{A}\right]\right|^2 + 2\left(\frac{6\|A\|}{K}\right)^2, \qquad \text{(A.26)}
\end{aligned}$$

where $\overline{\rho}_t = e^{-i\overline{H}t}\rho_t e^{i\overline{H}t}$ and $\overline{\omega}$ is the corresponding dephased state. This implies

$$\widetilde{\mathcal{D}}_A\left(\rho_t, \omega\right) \leq \frac{\|\overline{A}\|^2}{\|A\|^2}\widetilde{\mathcal{D}}_{\overline{A}}\left(\overline{\rho}_t, \overline{\omega}\right) + \frac{18}{K^2}. \qquad \text{(A.27)}$$

For the term $\widetilde{\mathcal{D}}_{\overline{A}}(\overline{\rho}_t, \overline{\omega})$ we can apply Propositions 4.1 and 4.2, and condition(i) to get

$$\begin{aligned}\left\langle \widetilde{\mathcal{D}}_{\overline{A}}(\overline{\rho}_t, \overline{\omega}) \right\rangle_T &\leq \frac{c\, a(\epsilon)\overline{Q}^2}{T\overline{\sigma}_G} + c\,\delta(\epsilon)\overline{Q}^2 \\ &\leq \frac{c\|\overline{A}\|^{1/2} a(\epsilon)\overline{Q}^{5/2}}{T\sqrt{\left|\mathrm{Tr}\Big(\big[\,[\rho_0, H]\,, H\big]\,A\Big)\right|}} + c\,\delta(\epsilon)\overline{Q}^2.\end{aligned} \tag{A.28}$$

The last inequality comes from our convenient construction of $\overline{\rho}_0$ and $\overline{A}$, specifically designed for this.

A.2.3 The factor $\overline{Q}$ for $\overline{\rho}_0$ and $\overline{A}$

It is easy to see that the factor $\overline{Q}$ for the auxiliary state and observable satisfies

$$\begin{aligned}\overline{Q} &\equiv \sum_{j\neq k} |\overline{\rho}_{jk}| \frac{|\overline{A}_{kj}|}{\|\overline{A}\|} \\ &= \sum_{jk\in J} |\rho_{jk}| \frac{|A_{kj}|}{\|\overline{A}\|} + 2\frac{|x|}{2}\frac{\|A\|}{2\|\overline{A}\|} \\ &= \frac{\|A\|}{\|\overline{A}\|}\left(Q_{\mathrm{trunc}} + \frac{|x|}{2}\right) \\ &\leq \frac{\|A\|}{\|\overline{A}\|}\left(Q_{\mathrm{trunc}} + \frac{2}{K}\right),\end{aligned} \tag{A.29}$$

where Q_{trunc} is the normalization constant of the distribution that results from $\Pi\rho_0\Pi$ and A.

The above bound, plus equations (A.27) and (A.28), result in

$$\begin{aligned}\left\langle \widetilde{\mathcal{D}}_A(\rho_t, \omega) \right\rangle_T &\leq \frac{\|\overline{A}\|^2}{\|A\|^2} \frac{c\, a(\epsilon)\|\overline{A}\|^{1/2}\overline{Q}^{5/2}}{T\sqrt{\left|\mathrm{Tr}\Big(\big[\,[\rho_0, H]\,, H\big]\,A\Big)\right|}} + \frac{\|\overline{A}\|^2}{\|A\|^2} c\,\delta(\epsilon)\overline{Q}^2 + \frac{18}{K^2} \\ &\leq \frac{c\, a(\epsilon)\|A\|^{1/2}\left(Q_{\mathrm{trunc}} + \frac{2}{K}\right)^{5/2}}{T\sqrt{\left|\mathrm{Tr}\Big(\big[\,[\rho_0, H]\,, H\big]\,A\Big)\right|}} + c\,\delta(\epsilon)\left(Q_{\mathrm{trunc}} + \frac{2}{K}\right)^2 + \frac{18}{K^2},\end{aligned} \tag{A.30}$$

which, defining $Q_2 = Q_{\mathrm{trunc}} + \frac{2}{K}$ to simplify notation, gives the first part of Theorem 4.10.

In order to finish the theorem's proof we upper bound Q_{trunc}. From eq. (4.16) on page 56

we see that for the truncated state

$$\begin{aligned} Q_{\text{trunc}}^2 &\leq \operatorname{Tr}\left[\left(\Pi\rho_0\Pi\right)^2\right] \operatorname{Tr}\left[\Pi\right] \\ &= \operatorname{Tr}\left[\Pi\rho_0\Pi\rho_0\right] d_{\text{trunc}} \\ &\leq \sqrt{\operatorname{Tr}\left[\Pi\rho_0^2\Pi\right] \operatorname{Tr}\left[\rho_0\Pi^2\rho_0\right]} d_{\text{trunc}} \\ &\leq \|\Pi\| \operatorname{Tr}\left[\rho_0^2\right] d_{\text{trunc}} \\ &= \operatorname{Tr}\left[\rho_0^2\right] d_{\text{trunc}}, \end{aligned} \tag{A.31}$$

by using that $d_{\text{trunc}} = \operatorname{Tr}\left[\Pi\right]$, the Cauchy-Schwarz inequality, and the fact that for two positive semidefinite matrices $\operatorname{Tr}\left[OP\right] \leq \|O\| \operatorname{Tr}\left[P\right]$.

Since $\rho_0 = \rho_S \otimes \frac{\mathbb{1}_B^\Delta}{d_B^\Delta}$ we see

$$\operatorname{Tr}\left[\rho_0^2\right] = \frac{\operatorname{Tr}_S\left[\rho_S^2\right]}{d_B^\Delta}. \tag{A.32}$$

Moreover, in the main text we found (see eq. (4.47) on page 66)

$$d_{\text{trunc}} \leq \frac{d_S d_B^\Delta}{\left(1-\frac{1}{K}\right)\left(1-e^{-\beta\Delta}\right)} e^{\beta\|H_S\| + \left(1+\sqrt{2d_s}\right)K\beta\|H_I\|}, \tag{A.33}$$

which leads to

$$\begin{aligned} Q_{\text{trunc}}^2 &\leq \operatorname{Tr}\left[\rho_0^2\right] d_{\text{trunc}} \\ &\leq \frac{d_S \operatorname{Tr}_S\left[\rho_S^2\right]}{\left(1-\frac{1}{K}\right)\left(1-e^{-\beta\Delta}\right)} e^{\beta\|H_S\| + \left(1+\sqrt{2d_s}\right)K\beta\|H_I\|}. \end{aligned} \tag{A.34}$$

Substituting this back into the definition for Q_2 gives eq. (4.51) on page 67, finishing the proof of Theorem 4.10.

A.2.4 Spin ring simulation

12/10/15 6:47 PM C:\Users\garciapi...\simulacionSpinRing.m 1 of 2

```
clear all

N=8                                                 %Size of the spin ring
gamma = 0.01                                        %Strength of the interaction

sigmaz = zeros(2,2,N);
sigmax = zeros(2,2,N);
auxz = [1, 0; 0, -1];
auxx = [0,1; 1,0];
for j=1:N
    sigmaz(:,:,j) = auxz;
    sigmax(:,:,j) = auxx;
end


%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%% INTERACTION HAMILTONIAN FOR A RING OF LENGTH N, sigmaX-sigmaX  %%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

Hint = zeros(2^N,2^N);
for j = 1:N-1
    Hint = Hint + kron( kron( eye(2^(j-1)), kron( sigmax(:,:,j),sigmax(:,:,j+1) ) ), eye↙
(2^(N-(j+1))) );
end
Hint = Hint + kron( kron( sigmaz(:,:,1),eye(2^(N-2)) ), sigmaz(:,:,1));        %To make↙
it a ring


%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%% SELF HAMILTONIAN FOR A CHAIN OF LENGTH N, sigmaZ %%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

H0 = zeros(2^N,2^N);
for j = 1:N-1
    H0 = H0 + kron( kron( eye(2^(j-1)),  sigmaz(:,:,j) ), eye(2^(N-j)) );
end


%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%             TOTAL HAMILTONIAN                                    %%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

H = H0 + gamma*Hint;
[V,D] = eig(H);                     %EIGENVALUES and EIGENVECTORS of H


%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%    BULDING THE INITIAL STATE and OBSERVABLE      %%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

rhosys = [1.0, 0.0; 0.0, 0.0];
```

```
rho = kron(rhosys, eye(2^(N-1))/2^(N-1));
Asys = sigmax(:,:,1);
A = kron(Asys, eye(2^(N-1)));


%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%                        Plotting p                              %%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

x = 1;
for n = 1:2^N
    for m = 1:2^N
        if n ~= m
        Gaux(x) = D(n,n)-D(m,m);
        G(x) = Gaux(x);
        paux(x) = abs( ( V(:,n)'*rho*V(:,m) )*( V(:,m)'*A*V(:,n) ) );
        x = x+1;
        end
    end
end
p = paux/sum(paux);
X = G;
Y = p;
[X,I] = sort(X);
Y = Y(I);

Nintervalos = 60;                   %Chose this to be EVEN
DX = (max(X)-min(X))/Nintervalos;
XBINNED = (min(X)+0.5*DX):DX:(max(X)-0.5*DX);
clear YBINNED
YBINNED = zeros(1,Nintervalos);
for K = 1:Nintervalos/2
    for j = 1:length(Y)
        if min(X) + (K-1)*DX <= X(j) && X(j) < min(X) + K*DX
            YBINNED(K) = YBINNED(K) + Y(j);
        end
    end
    K
    YBINNED(Nintervalos - (K-1)) = YBINNED(K)  %using that palpha distribution is↙
symmetric
end

norm = sum(YBINNED)*DX ;
YBINNED = YBINNED/norm ;

figure(1), bar(XBINNED,YBINNED,1,'FaceColor',[035 106 250]/255)
xlabel('energy gaps G')
ylabel('p(G)')
title('L = 8, \gamma = 0.01')
axis([-15 15 0 max(YBINNED)*1.1])
```

A.3 Environment in a typical state: Proposition 4.11

With the initial state

$$\rho_0^U = \rho_S \otimes U\left|\psi\right\rangle \left\langle\psi\right| U^\dagger = \rho_S \otimes \rho_B^U \tag{A.35}$$

we focus on the average over all unitaries U within the subspace $\mathcal{H}_{H_B}^{E_B,\Delta}$of $\widetilde{\mathcal{D}}_A\big(\rho_t^U,\omega^U\big)$:

$$\big\langle \widetilde{\mathcal{D}}_A\big(\rho_t^U,\omega^U\big)\big\rangle_U = \frac{\Big\langle \Big|\operatorname{Tr}\left[\rho_t^U A\right] - \operatorname{Tr}\left[\omega^U A\right]\Big|^2\Big\rangle_U}{4\|A\|^2}. \tag{A.36}$$

By shifting the time dependencies to the observable A we get

$$\operatorname{Tr}\left[\rho_t^U A\right] = \operatorname{Tr}\left[\rho_0^U e^{iHt} A e^{-iHt}\right] \equiv \operatorname{Tr}\left[\rho_0^U A(t)\right]. \tag{A.37}$$

If A_{eq} is the infinite time averaged $A(t)$, we have $\operatorname{Tr}\left[\omega^U A\right] = \operatorname{Tr}\left[\rho_0^U A_{eq}\right]$. Then

$$\begin{aligned}
\big\langle \widetilde{\mathcal{D}}_A\big(\rho_t^U,\omega^U\big)\big\rangle_U &= \frac{1}{4\|A\|^2}\left\langle \left|\operatorname{Tr}\left[\rho_0^U\left(A(t)-A_{eq}\right)\right]\right|^2\right\rangle_U \\
&= \frac{1}{4\|A\|^2}\Big\langle \Big|\operatorname{Tr}_B\left[\rho_B^U \operatorname{Tr}_S\left[\rho_S\otimes \mathbb{1}_B\big(A(t)-A_{eq}\big)\right]\right]\Big|^2\Big\rangle_U \\
&= \Big\langle \Big|\operatorname{Tr}_B\left[\rho_B^U C\right]\Big|^2\Big\rangle_U \\
&= \operatorname{Tr}_{B^{\otimes 2}}\left[\left\langle \rho_B^U\otimes\rho_B^U\right\rangle_U C\otimes C\right],
\end{aligned} \tag{A.38}$$

where in the third line we have used $\rho_B^U = \mathbb{1}_B^\Delta \rho_B^U \mathbb{1}_B^\Delta$ to write

$$C \equiv \frac{1}{2\|A\|}\operatorname{Tr}_S\left[\rho_S\otimes \mathbb{1}_B^\Delta\big(A(t)-A_{eq}\big)\mathbb{1}_S\otimes\mathbb{1}_B^\Delta\right] \tag{A.39}$$

as an observable acting on the microcanonical window of the bath Hilbert space.

Lemma 3.5 on page 41 gives

$$\begin{aligned}
\left\langle \rho_B^U\otimes\rho_B^U\right\rangle_U &= \Big\langle U^{\otimes 2}\Big(\left|\psi\right\rangle\left\langle\psi\right|\otimes\left|\psi\right\rangle\left\langle\psi\right|\Big)\left(U^{\otimes 2}\right)^\dagger\Big\rangle_U \\
&= \alpha\Pi_s + \beta\Pi_a,
\end{aligned} \tag{A.40}$$

where $\Pi_s = \frac{(\mathbb{1}_B^\Delta)^{\otimes 2}+\$}{2}$ and $\Pi_a = \frac{(\mathbb{1}_B^\Delta)^{\otimes 2}-\$}{2}$, and $\$$ is the swap operator on $\mathcal{H}_{H_B}^{E_B,\Delta}\otimes\mathcal{H}_{H_B}^{E_B,\Delta}$,

defined by $\$ \left|\phi_1\right\rangle \left|\phi_2\right\rangle = \left|\phi_2\right\rangle \left|\phi_1\right\rangle$. Since

$$\begin{aligned}\mathrm{Tr}\left[\left\langle \rho_B^U \otimes \rho_B^U \right\rangle_U \Pi_a\right] &= \frac{1}{2}\Big\langle \left(1 - \mathrm{Tr}\left[\rho_B^U \otimes \rho_B^U \,\$\right]\right) \Big\rangle_U \\ &= \frac{1}{2}\Big\langle \left(1 - \mathrm{Tr}\left[(\rho_B^U)^2\right]\right) \Big\rangle_U \\ &= 0 \end{aligned} \tag{A.41}$$

we see that $\beta = 0$, and from $\mathrm{Tr}\left[\left\langle \rho_B^U \otimes \rho_B^U \right\rangle_U\right] = 1$ we obtain $\alpha = \frac{2}{d_B^\Delta (d_B^\Delta + 1)}$, which leads to the simple expression $\left\langle \rho_0^U \otimes \rho_0^U \right\rangle_U = \frac{2}{d_B^\Delta (d_B^\Delta + 1)} \Pi_s$. Then

$$\begin{aligned}\left\langle \widetilde{\mathcal{D}}_A\big(\rho_t^U, \omega^U\big) \right\rangle_U &= \frac{2}{d_B^\Delta (d_B^\Delta + 1)} \mathrm{Tr}_{B^{\otimes 2}}\left[\Pi_s C \otimes C\right] \\ &= \frac{1}{d_B^\Delta (d_B^\Delta + 1)} \Big(\mathrm{Tr}_{B^{\otimes 2}}\left[(\mathbb{1}_B^\Delta)^{\otimes 2} C \otimes C\right] + \mathrm{Tr}_{B^{\otimes 2}}\left[\$\, C \otimes C\right] \Big) \\ &= \frac{1}{d_B^\Delta (d_B^\Delta + 1)} \Big(\mathrm{Tr}_B\left[C\right]^2 + \mathrm{Tr}_B\left[C^2\right] \Big). \end{aligned} \tag{A.42}$$

The operator C is of the form $C = \mathrm{Tr}_S[O]$, with O Hermitian and acting only on the microcanonical window, from its definition above. Any such operator can be written as

$$O = \sum_{j=0}^{d_S^2 - 1} \sum_{k=0}^{\left(d_B^\Delta\right)^2 - 1} a_{jk} X_j Y_k \tag{A.43}$$

where a_{jk} are real coefficients, and $\{X_j\}$ and $\{Y_k\}$ are orthonormal bases of Hermitian operators on system and microcanonical window respectively [56]. They satisfy

$$\begin{aligned}&\mathrm{Tr}_S\left[X_j X_{j'}\right] = \delta_{jj'}, \quad \forall \{j, j'\} = \left(0, \dots d_S^2 - 1\right) \\ &\mathrm{Tr}_B\left[Y_k Y_{k'}\right] = \delta_{kk'}, \quad \forall \{k, k'\} = \left(0, \dots (d_B^\Delta)^2 - 1\right), \end{aligned} \tag{A.44}$$

$X_0 = \frac{\mathbb{1}_S}{\sqrt{d_S}}$ and $Y_0 = \frac{\mathbb{1}_B^\Delta}{\sqrt{d_B^\Delta}}$, while all other operators have trace 0. With these definitions we

can write

$$\begin{aligned}
\mathrm{Tr}_B\left[C^2\right] &= \mathrm{Tr}_B\left[\mathrm{Tr}_S\left[O\right]\mathrm{Tr}_S\left[O\right]\right] \\
&= \sum_{jj'=0}^{d_S^2-1}\sum_{kk'=0}^{\left(d_B^\Delta\right)^2-1} a_{jk}a_{j'k'}\,\mathrm{Tr}_B\left[\mathrm{Tr}_S\left[X_j\right]\mathrm{Tr}_S\left[X_{j'}\right]Y_kY_{k'}\right] \\
&= \sum_{kk'=0}^{\left(d_B^\Delta\right)^2-1} a_{0k}a_{0k'}\,\mathrm{Tr}_B\left[Y_kY_{k'}\right]\mathrm{Tr}_S\left[X_0\right]\mathrm{Tr}_S\left[X_0\right] \\
&= d_S\sum_{kk'=0}^{\left(d_B^\Delta\right)^2-1} a_{0k}a_{0k'}\delta_{kk'} = d_S\sum_{k=0}^{\left(d_B^\Delta\right)^2-1} a_{0k}^2 \\
&\leq d_S\sum_{j=0}^{d_S^2-1}\sum_{k=0}^{\left(d_B^\Delta\right)^2-1} a_{jk}^2 = d_S\,\mathrm{Tr}\left[O^2\right].
\end{aligned} \tag{A.45}$$

From this result, and the definition of C above,

$$\begin{aligned}
\mathrm{Tr}_B\left[C^2\right] &\leq \frac{d_S}{4\|A\|^2}\,\mathrm{Tr}\left[(\rho_S\otimes\mathbb{1}_B^\Delta\big(A(t)-A_{eq}\big))^2\right] \\
&\leq \frac{d_S}{4\|A\|^2}\sqrt{\mathrm{Tr}\left[(\rho_S\otimes\mathbb{1}_B^\Delta)\big(A(t)-A_{eq}\big)^2(\rho_S\otimes\mathbb{1}_B^\Delta)\right]} \\
&\qquad\times\sqrt{\mathrm{Tr}\left[\big(A(t)-A_{eq}\big)(\rho_S\otimes\mathbb{1}_B^\Delta)^2\big(A(t)-A_{eq}\big)\right]} \\
&\leq \frac{d_S}{4\|A\|^2}\,\mathrm{Tr}\left[(\rho_S\otimes\mathbb{1}_B^\Delta)^2\right]\|A(t)-A_{eq}\|^2 \\
&\leq d_Sd_B^\Delta
\end{aligned} \tag{A.46}$$

by using Cauchy-Schwarz inequality on line 2, the fact that for positive semidefinite operators $\mathrm{Tr}\left[OP\right]\leq\mathrm{Tr}\left[O\right]\|P\|$ on line 3, and the triangle inequality plus $\|A_{eq}\|\leq\|A(t)\|=\|A\|$ on the last line.

With this result we see that eq. (A.42) turns into

$$\begin{aligned}\left\langle \widetilde{\mathcal{D}}_A\big(\rho_t^U,\omega^U\big)\right\rangle_U &= \frac{1}{d_B^\Delta(d_B^\Delta+1)}\left(\mathrm{Tr}_B\left[C\right]^2+\mathrm{Tr}_B\left[C^2\right]\right)\\ &\leq \frac{1}{d_B^\Delta(d_B^\Delta+1)}\left(\frac{1}{4\|A\|^2}\,\mathrm{Tr}\left[\rho_S\otimes \mathbb{1}_B^\Delta\big(A(t)-A_{eq}\big)\right]^2+d_S d_B^\Delta\right)\\ &= \frac{1}{d_B^\Delta(d_B^\Delta+1)}\left(\frac{(d_B^\Delta)^2}{4\|A\|^2}\,\mathrm{Tr}\left[\rho_S\otimes \frac{\mathbb{1}_B^\Delta}{d_B^\Delta}\big(A(t)-A_{eq}\big)\right]^2+d_S d_B^\Delta\right)\\ &= \frac{d_B^\Delta}{d_B^\Delta+1}\frac{\mathrm{Tr}\left[\rho_0\big(A(t)-A_{eq}\big)\right]^2}{4\|A\|^2}+\frac{d_S}{d_B^\Delta+1},\end{aligned} \tag{A.47}$$

where $\rho_0\equiv\rho_S\otimes\frac{\mathbb{1}_B^\Delta}{d_B^\Delta}$. We can now shift the time dependence back to the state to get

$$\begin{aligned}\left\langle \widetilde{\mathcal{D}}_A\big(\rho_t^U,\omega^U\big)\right\rangle_U &\leq \frac{d_B^\Delta}{d_B^\Delta+1}\frac{\mathrm{Tr}\left[(\rho_t-\omega)\,A\right]^2}{4\|A\|^2}+\frac{d_S}{d_B^\Delta+1}\\ &\leq \frac{\mathrm{Tr}\left[(\rho_t-\omega)\,A\right]^2}{4\|A\|^2}+\frac{d_S}{d_B^\Delta}\\ &= \widetilde{\mathcal{D}}_A\big(\rho_t,\omega\big)+\frac{d_S}{d_B^\Delta},\end{aligned} \tag{A.48}$$

which proves our claim. The bound $\frac{1}{d_B^\Delta+1}\leq\frac{1}{d_B^\Delta}$ is only for presentation reasons and does not change the result much since $d_B^\Delta\gg d_S>1$ in the regime we are interested in.

A.4 Gaussian channels with finite distillable work

Let Ω be a Gaussian channel whose action on the displacement vector $\vec{d}$ and covariance matrix γ of the m-mode input state is given by

$$\vec{d} \to X\vec{d} + \vec{z}, \qquad \gamma \to X\gamma X^T + Y. \tag{A.49}$$

Suppose that Ω acts on a system with Hamiltonian $H = \vec{R}^T G \vec{R} + \vec{h} \cdot \vec{R}$, where $\vec{R}$ is the vector of optical quadratures. Under the assumption that $\tilde{G} \equiv G - X^T G X > 0$, we wonder if the difference between the free energies of the input and output states is bounded, i.e., whether $\Delta F(\rho, \Omega) < K$, for some $K < \infty$.

Call E_0 the energy of the input state, and γ and $\vec{d}$, its covariance matrix and displacement vector. Then we have that

$$E_0 = \frac{1}{2} \operatorname{Tr}[G\gamma] + (\vec{d} - \vec{d_0})^T G (\vec{d} - \vec{d_0}) - \bar{E}, \tag{A.50}$$

where $\vec{d_0} \equiv -G^{-1}\vec{h}/2$ and $\bar{E} \equiv \vec{d_0}^T G \vec{d_0}$. Hence, defining $\mu_{\min} > 0$ and $\mu_{\max} > 0$ to be the minimum and maximum eigenvalue of G respectively, we have that

$$\frac{E_0 + \bar{E}}{\mu_{\max}} \leq \left(\frac{1}{2} \operatorname{Tr}[\gamma] + \|\vec{d} - \vec{d_0}\|^2 \right) \leq \frac{E_0 + \bar{E}}{\mu_{\min}}, \tag{A.51}$$

and consequently

$$\begin{aligned} &\operatorname{Tr}[\gamma] \leq \mathcal{O}(E_0), \quad \|\vec{d}\| \leq \mathcal{O}(\sqrt{E_0}), \\ &\frac{1}{2} \operatorname{Tr}[\gamma] + \|\vec{d} - \vec{d_0}\|^2 \geq \mathcal{O}(E_0). \end{aligned} \tag{A.52}$$

We can now bound the energy difference between the input and output states. First, note that $\Delta E \equiv E_f - E_0$ can be written as:

$$\Delta E = -\frac{1}{2} \operatorname{Tr}\left[\gamma \tilde{G}\right] - (\vec{d} - \vec{d_0})^T \tilde{G} (\vec{d} - \vec{d_0}) + \mathcal{O}(\vec{d}). \tag{A.53}$$

Defining $\lambda_{\min} > 0$ to be the smallest eigenvalue of $\tilde{G}$, we thus arrive at

$$\begin{aligned}\Delta E &\leq -\lambda_{\min}\left(\frac{1}{2}\operatorname{Tr}[\gamma] + \|\vec{d} - \vec{d_0}\|^2\right) + \mathcal{O}(\vec{d}) \\ &\leq -\mathcal{O}(E_0) + \mathcal{O}(\sqrt{E_0}) = -\mathcal{O}(E_0).\end{aligned} \tag{A.54}$$

Let us now bound the entropy of the input state: by the subadditivity of the von Neumann entropy, $S(\rho)$ is bounded from above by $\sum_{j=1}^{m} S(\rho_j)$, where ρ_j denotes the reduced density matrix of each mode j. In turn, $S(\rho_j)$ is upper bounded by the von Neumann entropy of the Gaussian state with the same first and second moments as ρ_j, i.e., a Gaussian state with covariance matrix γ_j [106]. Note that $\sum_{j=1}^{m} \operatorname{Tr}[\gamma_j] = \operatorname{Tr}[\gamma] \leq \mathcal{O}(E_0)$, where the last inequality is due to eq. (A.52). In particular, $\operatorname{Tr}[\gamma_i] \leq \mathcal{O}(E_0)$ for $j = 1, ..., m$.

The entropy of a 1-mode Gaussian state with covariance matrix $\tilde{\gamma}$ is given by eq. (5.43) on page 92,

$$S = (N+1)\log(N+1) - N\log(N) = \mathcal{O}(\log(N)), \tag{A.55}$$

where $N = \sqrt{\det(\tilde{\gamma})}$. For any 2×2 matrix A it holds that $\det(A) \leq (\operatorname{Tr}[A])^2$, hence $N \leq \operatorname{Tr}[\tilde{\gamma}]$. It follows that

$$S(\rho) \leq \mathcal{O}(\log(E_0)). \tag{A.56}$$

Putting all together, we have that

$$\begin{aligned}\Delta F(\rho, \Omega) &\leq \Delta E + K_B T S(\rho) \\ &\leq -\mathcal{O}(E_0) + \mathcal{O}(\log(E_0)).\end{aligned} \tag{A.57}$$

The last expression cannot thus take arbitrarily large values, and so the distillable work of channel Ω is bounded.

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