# Non-equilibrium fluctuations and athermality as quantum resources

**By**

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I, Alvaro Martin Alhambra, confirm that the work presented in this thesis is my own. Where information has been derived from other sources, I confirm that this has been indicated in the thesis.

Signed ............................................ Date ................

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## Abstract

Within quantum information, a very productive way to look at physical phenomena is under the light of the framework of resource theories. Through it, one can focus on questions such as in what sense a particular physical feature can be thought of as a resource for certain tasks, and how can it be quantified. A particularly prominent example of this is the theory of quantum entanglement.

In recent years, a research program has emerged in which researchers are trying to build a resource theory relevant for thermodynamical and non-equilibrium phenomena at the quantum and nano scales. The overarching aim is to find how the perspective given by quantum information tools and techniques help us understand new and existing results of the field. In this thesis we advance these efforts by introducing different kinds of non-equilibrium fluctuations into the theory: fluctuations of work and fluctuations of states. In this way, we manage to merge a number of ideas from the field of stochastic thermodynamics into the resource-theoretic framework. We further explore the structure of this resource theory by introducing results in which the finiteness of the heat bath's size is considered, deriving corrections to well-known expressions regarding work extraction. On top of this, we also consider the usefulness within non-equilibrium thermodynamics of other tools coming from quantum information theory, such as the relative entropy and the idea of a recovery map. The connection between the recovery map and the property of quantum detailed balance (and time reversal more generally) is highlighted, and a bound on the entropy production of Davies maps is derived inspired by recent results on quantum information.

# List of Publications and Preprints

The work presented in this thesis contains material from the following publications:

Álvaro M Alhambra, Jonathan Oppenheim, and Christopher Perry. *Fluctuating States: What is the Probability of a Thermodynamical Transition?* Physical Review X, 6(4):041016, 2016.

Álvaro M Alhambra, Lluis Masanes, Jonathan Oppenheim, and Christopher Perry. *Fluctuating Work: From Quantum Thermodynamical Identities to a Second Law Equality* Physical Review X, 6(4):041017, 2016.

Álvaro M Alhambra and Mischa P Woods. *Dynamical maps, quantum detailed balance and the Petz recovery map.* Physical Review A, 96(2):022118, 2017.

Jonathan G Richens, Álvaro M Alhambra, and Lluis Masanes. *Finite-bath corrections to the second law of thermodynamics.* arXiv preprint arXiv:1702.03357, 2017.

Other preprints by the author are:

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*I have been asking myself whether natural forms - a tree, a cloud, a river, a stone, a flower - can be looked at and perceived as messages. Messages - it goes without saying - which can never be verbalized, and are not particularly addressed to us. Is it possible to 'read' natural appearances as texts? For me there is nothing mystical in this exercise. It is a gestural exercise, whose aim is to respond to different rhythms and forms of energy, which I like to imagine as texts from a language that has not been given to us to read. Yet as I trace the text I physically identify with the thing I'm drawing and with the limitless, unknown mother tongue in which it is written.*

- John Berger in "How To Resist A State Of Forgetfulness"

# Introduction

Physical systems in our macroscopic experience are always found to have thermodynamical properties such as temperature, pressure or magnetization and depending on them, different energy flows are found to occur. Examples are the flow of energy from a hot coffee into air, or the opposite flow from a fridge to its contents.

The basic theoretical foundations of these fundamental features of nature go back to the 19th century and the origin of statistical mechanics by Gibbs, Boltmann, Maxwell and others. The key general idea behind these breakthroughs was to understand thermodynamical phenomena as the collective behaviour arising from the effective stochasticity of the microscopic components of macroscopic matter.

What is exactly the origin of this effective stochasticity? The shortest answer is that it is due to macroscopic observers not having full access to the microscopic degrees of freedom, which are hence forced into a coarse-grained description. Reasonable assumptions such as maximum entropy principles or ergodicity lead to the emergence of thermodynamical ensembles after that coarse-graining is made. These in turn are the statistical ensembles that give rise to the thermodynamics of macroscopic systems at equilibrium. The foundations of this subject are still a matter of discussion, and a proper justification for those “reasonable assumptions” has not been established to the level of rigour and generality that some people demand. As famously put by Uffink [179], “statistical physics, however, has not yet developed a set of generally accepted formal axioms”.

Along those lines, for instance, a lot of research efforts are nowadays focused on showing how thermal ensembles appear in many-body quantum dynamics [76, 77]. In any case, as far as more practical matters are concerned, the theory of equilibrium thermodynamics is now one of the most basic pillars of physics, and is studied with different levels of depth in most physical sciences and engineering university degrees.

When we have access to individual small systems, however, things become more interesting and we can find a lot more questions that have not yet been answered. At small scales, the effective stochasticity is such that non-equilibrium physics plays a bigger role, and this opens the door to a lot more structure and a richer variety of phenomena. This is because in this context we aim to describe a more reasonable number of degrees of freedom than in macroscopic thermodynamics (of an order much smaller than $10^{23}$), and the non-equilibrium behavior becomes potentially more tractable.

The field of modern stochastic and non-equilibrium thermodynamics aims to explore the regimes of these small scales, where statistical fluctuations are very important, and concepts such as work and heat become a lot more elusive. This is still today a very active field of research, with an ever-growing interest motivated by our increased ability to control small systems (see [160, 9, 78, 186] for various reviews). A non-exhaustive list of the aims of this field is

- Understand the key general features of non-equilibrium behaviour. Part of this entails giving quantitative statements of the irreversibility of these processes, and of the second law of thermodynamics. A notable example are the *fluctuation theorems*, which we will describe thoroughly along the text (see [41, 63] for reviews on this).

- In relation to macroscopic thermodynamics, to give a more solid microscopic foundation to the origin of the thermal ensembles, both canonical and microcanonical. On top of that, understand the circumstances under which we do not expect those ensembles to appear, such as in integrable systems [51].

- Explore the ways of properly accounting for the flows of energy and entropy between small systems. This involves the subtle question of identifying transport currents, and flows of heat and work, concepts that seem to be notoriously hard to define in general [13, 172, 81, 75, 73], specially when phenomena like strong coupling or non-markovianity are present [167, 138, 181].

- As far as practical applications are concerned, the benefits may come via finding schemes and implementations for efficient microscopic heat engines or refrigerators [14, 74, 111, 55, 131]. A particularly interesting question has to do with whether and how do genuine quantum effects such as coherence or entanglement help boost their performance (see [36, 128, 56, 180, 104] for results along this direction).

Indeed, as one probes increasingly smaller scales, the regimes where quantum effects can become important are reached. Nature is ultimately quantum, and for that simple reason it must be that, when looking at a sufficiently small scale, the stochasticity of any natural process comes from quantum effects. However, we only expect to see these clearly for certain systems with sizes and actions of the order of the quantum scale, where decoherence and other phenomena do not yet hinder their appearance. When this happens, an extra level of complexity and richness of physical structure is introduced, and new tools are needed.

This is the point where the field of quantum information theory comes into play. Seminal results such as the no-cloning theorem [137, 195] or the first quantum cryptographic protocols [23] hinted at the fact that perhaps thinking of the quantum description of systems as a different kind of information was a productive way of understanding problems in physics. This kind of information is different to the "classical" one because it cannot be cloned, and because the kind of correlations it creates between systems are fundamentally different to the classical ones. After the idea of quantum computing appeared, and specially with the explosion subsequent to the discovery of Shor's algorithm for factoring numbers, the field has grown and is now a very important branch of physics, whose influence is already notable in areas such as atomic physics, condensed matter physics or high energy physics.

Given that quantumness must at some point play a role in the non-equilibrium behaviour of small systems, it is expected that another field where quantum information can offer positive insights is non-equilibrium statistical physics. The results in this thesis are a small part of the efforts from quantum information theorists to break into that realm, with the aim of finding new ideas and perspectives that may be otherwise obscured by more traditional approaches.

## 0.1 The idea of a (quantum) resource theory

A big overarching target of quantum information has to do with how we understand and quantify the true *quantumness* of the systems at hand. As a most prominent example, going back to the seminal work of Bell [20], we know that entanglement is a feature of nature that cannot appear in the classical world. After that, some important results in entanglement theory, specially starting in the early and mid 90's, such as the concept of entanglement distillation and entanglement entropy [22, 24], quantum cryptography via Bell's theorem [62] or the theory of quantum communication [157, 158, 112, 91] made it clear that it could be understood as a truly quantum *resource*.

The theory behind how entanglement can be manipulated, quantified, or used in practical applications, has been an extremely active field of research since then. A lot is now known about the structure of the set of entangled states, in a field that one can name the *resource theory of entanglement*. A definitive review of this field is [92].

With this extremely rich resource theory in mind, a natural question to ask was whether one can build a resource theory of some other physical property other than entanglement. One reason why this may be the case is that a lot of evidence shows that entanglement is not the only truly quantum resource useful for all informational tasks. This is already evident if one looks, for instance, at the original BB84 cryptographic protocol [23], which does not require entanglement, but quantum coherence only. On top of that, from the idea of entanglement as a resource one can easily extrapolate which are the elements that can make up a resource theory. This way one can build a general template for further examples of such theories [90, 30, 45].

But what is exactly a resource theory? From the template of entanglement, we can define it as an abstract theoretical framework whose building blocks are the following elements:

- The set of *free states*, to which no resource value is attributed. In entanglement, these are states which can be prepared with local operations and classical communication, the so-called *separable* states. The result of [163] are an exception to this rule: they define a thermodynamic resource theory in which thermal states are not a free resource.

- A set of *free operations*, which by definition do not generate a resource. This means, at least, that they take a state from the set of free states to another state within that set.

- A set of quantifiers, which give information about the particular value of different instances of a resource. Quite often these take the form of *monotones*, which are scalar functions of quantum states that can only decrease when a free operation is applied to the quantum state at hand. In entanglement, some of these can be thought of as the distance of a given entangled state to the set of separable states [183].

Examples of resource theories that fit into this description are, for instance, the theory of reference frames [18] and the closely related *asymmetry* theory [123, 120], quantum coherence [168], stabilizer quantum computation [184] or purity [80]. Studying the structure of any one of these theories is a program that can be separated in two different stages:

i) First, one has to motivate and define which are the right sets of free states or free operations, a choice that may in some cases be obvious, but that in some others causes a certain amount of discussion. For instance, one can define the free operations via some meaningful physical restriction, such as not having access to a quantum channel between Alice and Bob (LOCC), or one can define the strictly bigger set of operations that map free states to free states [33]. A timely example of a theory in which the different definitions are being discussed is the resource theory of coherence [122].

ii) Second, identify the relevant quantifiers, and derive the conditions under which different states can be transformed into each other via the free operations, and resources that need to be accounted for. Given this point, a resource theory can be understood as a theory about control: given a certain set of physical operations and resources, which kinds of states can be accessed from others? And which ones cannot?

A very natural question one can now ask is: can we build a meaningful quantum resource theory that may be relevant for non-equilibrium statistical physics? Two preliminary reasons why such an idea may make sense are:

- Classical equilibrium thermodynamics can be understood as a control theory. The following quote from David Wallace's article "Thermodynamics as control theory" [188] is enlightening in that respect:

  > [Thermodynamics] is not in the business of telling us how equilibrium states evolve if left to themselves, except in the trivial sense that they do not evolve

> at all: that is what equilibrium means, after all. When the states of thermodynamical systems change, it is because we do things to them: we put them in thermal contact with other systems, we insert or remove partitions, we squeeze or stretch or shake or stir them. And the laws of thermodynamics are not dynamical laws like Newton's: they concern what we can and cannot bring about through these various interventions.

Indeed, classical thermodynamics can be understood as the theory that describes how different equilibrium states of a system are interconnected through processes such as adiabats and isotherms. It is in that sense that we can think of it as a theory with a flavour similar to that of resource theories. The resource theory described in this thesis can be thought of as a generalization of such a control theory, in which we incorporate processes beyond the macroscopic, equilibrium-specific ones.

- Quantum resource theories, and entanglement in particular, have a very thermodynamical flavor to them, as the question of which states can be accessed from which others is (at least qualitatively) very reminscent of the content of the second law.

  For instance, a groundbreaking result by Nielsen [132] in the theory of pure bipartite entanglement established that the conditions for knowing when can one access one pure bipartite state from another are the *majorization* conditions. These conditions, which we will describe in detail in Chapters 1 and 2, make up a particular way of measuring how uniform a probability distribution is. In this sense, they are very closely connected to athermality.

  Another finding along these lines was [33], where the authors showed that in the many copies limit, a particular relative entropy (resemblant to a free energy) is the key measure in establishing when one can go from one mixed entangled state to another. Moreover one can define thermodynamics-based entanglement measures such as those found in [135]

  On top of that, a number of ideas from quantum information theory look like they may be useful in thermodynamics. For instance, with the development of quantum cryptography, researchers realised that measures of disorder other than the Shannon and von Neumann entropies are the relevant ones in secret key generation [148]. A natural question we will answer partially is whether these further measures are useful in characterizing athermality.

The construction of such a resource theoretic framework has been a very active research line within the field of quantum information theory, and rapid progress on a few fronts has been made. The contents of this thesis are embedded within this program and build on the initial efforts of works such as [93, 66, 60, 50, 1, 29, 89, 28], where the foundations of the resource theory of athermality were laid out, and a big amount of its important features were understood.

## 0.2 What do we expect to learn from this?

The field of statistical and non-equilibrium physics is a fairly old and vast one, so a fair question to ask why do we need a new quantum information based approach and in which way may a new set of ideas be useful.

Looking at past experience, the trend seems to be that whenever there is a successful combination of information theory and physics, the former gives a new perspective on the latter, and new useful concepts appear. This can translate into two different kinds of advances:

- A more precise understanding of existing phenomena. A very prominent example of this is the seminal idea of Hayden and Preskill on black hole physics [85], where they showed that if one understands black holes as optimal encoders of quantum information, or *scramblers* a great deal of their semiclassical behaviour (such as the entanglement between the interior and the exterior at most times) can be understood without resorting to quantum gravity, an idea which has sparked an enormous amount of new research in high energy physics. Another notable example is the understanding of quantum many body systems, with ideas such as entanglement entropy or area law scalings, that were brought into a stronger footing through quantum information results [83, 61].

- A better understanding of the information-theoretic and computational capabilities of systems, and of fundamental protocols that pave the way for practical applications. A very good example of this is how the early seminal results of quantum information, such as teleportation or entanglement distillation, have provided the building blocks for the quantum technologies being developed in the present.

The questions of importance for us are then the following: What is it that quantum information can help us understand in regards to non-equilibrium and statistical physics? And what kind of applications could we be looking for? Potential answers to these are:

- A deeper understanding of the role of information in thermodynamics. In that sense, the resource theory approach can be seen as building dramatically on Landauer's seminal idea connecting thermodynamical work and information [107].
- A definition and motivation of new information-theoretic ways of measuring athermality and non-equilibrium. This can happen, for instance, via the information-theoretic monotones which we will describe in Chapter 1. In fact, the same way as quantum entropies are motivated by coding theorems that limit how well messages can be sent down different kinds of channels, we can devise thermodynamics-like coding theorems, such as those in [29, 162, 163] that establish fundamental limitations to thermodynamical phenomena.
- Related to the point on coding theorems, more in general we want to explore the fundamental limitations for thermodynamical processes. That is, give means for knowing when particular transitions between states are possible. This amounts to answering what kinds of transitions between states are possible given a certain set of thermodynamical operations.
- Following from that, understand the limitations of hard tasks such as cooling [124, 192], and find efficient ways of doing it [35]. The results of the resource theory may be useful in, for instance, providing more efficient ways of *algorithmic cooling* [153, 136], as has been hinted in [114].
- Understanding the relevance of the truly quantum resources, such as coherence and entanglement. A pressing question in the foundations of thermodynamics is how do quantum effects appear in the theory, and how do they hinder or enhance different tasks. Results along these lines include, mostly regarding coherence, are for instance [49, 115, 116]. It is indeed believed that the resource theory provides a very clear theoretical framework for analyzing such questions.
- In a way similar to how the framework allows for analyzing the quantum resources, it

may also provide a good way of accounting for the thermodynamical costs of feedback [156] and control in quantum processes [194].

By now, after the relatively large body of work aimed at understanding the resource theory framework, we have a good grasp of a number of the key theoretical questions, in particular regarding the fundamental limitations of thermodynamical processes [89, 116, 117]. However, a number of issues along those lines have not up to date been answered, and most of the work in this thesis will be pushing in that direction.

A very common criticism towards the resource-theoretic approach is that it has not yet to this point given new predictions or insights regarding particular physical systems, or particular thermodynamical protocols that may be useful, and that hence some of the key aims we outline above are far from having been realized. We will not be addressing these issues very thoroughly here, but for progress along these lines, we refer the reader to, for instance, [141, 114].

## 0.3 Where is this thesis placed exactly?

As mentioned above, we are at a point where the theoretical framework of the resource theory has already been outlined and a lot of its structure is already known, in particular regarding general transitions between quasiclassical states, but there are quite a few pieces still missing from the global picture.

The framework of resource theories aims to be as general as it possibly can. Thus one of the challenges we face is to be able to incorporate results and ideas from traditional stochastic thermodynamics into the framework. Up to date, this had not been addressed properly in the literature, and some of the results of this thesis aim to solve that. In particular, we will be focusing on the idea of fluctuating work, and on the very well known fluctuation theorems. The results of Chapter 3 contain some of the first results in which work fluctuations are incorporated into the resource-theoretic framework.

The other two programs to which the results of this thesis contribute are

- Explore the structure of the resource theory formalism and the fundamental limitations it imposes. This amounts to answering questions such as what kind of transitions are possible under certain sets of operations, or the way in which different resources (in particular, work) are useful in enhancing their power. The results from Chapters 1, 2 and 3 go along those lines.

- Show particular ways in which tools from quantum information theory may be useful in non-equilibrium physics. One good example are the Renyi divergences or relative entropies, as we will explain in Chapter 1. A further example introduced here in Chapter 4 is related to the quantum-informational idea of a *recovery map*. We will see this appears naturally when talking about reversed processes in thermodynamics. These gives an idea for combining results in both fields in a way that they feed positively into each other.

# Guide to the contents of this thesis

## 0.4 Notation

We will be working in units for which the Boltzmann constant is $k_B = 1$, and also $\hbar = 1$.

Throughout this thesis we will be labelling Hamiltonians with the letter $H$ and partition functions as $Z$ with subindices $S, W, B$ indication whether they correspond to system, bath or weight. These physical systems will be in Hilbert spaces which we label as $\mathcal{H}_i$, and $\mathcal{S}(\mathcal{H}_i)$ will be the set of quantum states (that is, density matrices) belonging to that Hilbert space, $i$ being the particular subindex $S, W, B$. On top of that, unitary operators will be represented as $U$, with $U^\dagger U = \mathbb{I}$ being the identity on the Hilbert space on which $U$ acts.

We will refer throughout to a particular kind of maps (or channels) from one Hilbert space to another as *quantum* maps. We shall take this name as equivalent to CPTP map, which represents the most general kind of quantum evolution [133]. These maps are linear, completely positive and trace-preserving. They will usually be represented by a capital letter, usually $T$ or $M$, except for particular ones such as the decoherence map $\Delta$.

Quantum states, whether quasiclassical or not, will be labelled by the letters $\rho$ and $\sigma$, representing their density matrices. Generally we will take $\rho$ to be the input of a process, and $\sigma$ to be the output. Thermal states will be defined with the letter $\tau$ with a subindex $\beta$ to indicate the temperature that defines them, or, where ambiguous, with a subindex indicating whether they are the thermal state of system, bath or weight.

When the quantum states are quasiclassical (diagonal in the energy eigenbasis) they can be represented by a probability distribution. We will write them as $p_i$ and $q_j$, where $i, j$ label the individual initial and final energy levels.

Stochastic processes will be represented by conditional probabilities $P(j|i)$, $i$ being the random variable we condition on and $j$ the outcome of the process. In the *reversed processes*, the roles of $i$ and $j$ will be switched. When the work fluctuates, the work random variable will be represented by the letter $w$, while for deterministic work it will be written as $W$.

## 0.5 Structure and contents

We now outline the contents and the structure of the thesis, chapter by chapter.

In Chapter 1 we introduce the main ingredients of the resource theory, such as the free operations, the free resources and the monotones. The discussion will largely follow from the results from the works [29, 28, 115], and specially [89]. Throughout the chapter, however, we merge the results of those works with the original ones found in the author's work [149], in which a heat bath of finite size is imposed. Thus, the results of that section regarding the finiteness of the bath are original work from the author and collaborators.

Once the resource theoretic framework has been laid out, we start by expanding its scope with the results of Chapter 2, which is mostly based on the work [6]. There, a new kind of probabilistic thermodynamical transitions is considered, and results regarding the fundamental limitations of such transitions, and their relation to the work in the infinite bath limit, are laid out. The results, which build up specially from those on [185, 80, 89], were discovered by the author in collaboration with one of the coauthors and their supervisor.

Then we move to Chapter 3, in which the topic of work fluctuations is introduced. The results are based on [5], which constitutes one of the first efforts to include work fluctuations within the resource-theoretic framework (other relevant recent papers being for instance [75, 3]). We give a potential definition for work in this setting, and show that many of the fluctuation theorems that appear in the statistical physics literature can be derived from it. This constitutes a step forward in the ongoing task of bridging the results from the two fields together. The author participated in all of the results included in the chapter, and a technical proof worked out by another coauthor is placed in the appendix.

The last chapter is on a slightly different but related topic. It is largely based on [8] by the author and a collaborator, and on some key proofs of [7], although the initial discussion includes ideas from [64, 144], and a growing body of quantum information literature such as

[108, 190, 170, 169]. In that chapter, we introduce the quantum informational idea of a recovery map, and motivate in which way it may be related to the purely thermodynamical notion of entropy production. We then specialize in a kind of thermodynamical processes called Davies maps, which can be thought of as the set of Markovian thermal operations. The results regarding these evolutions essentially illustrate the way in which the quantum informational concept of a recovery map appears in the context of thermal equilibration, and shows an explicit connection between recoverability of information and thermodynamical reversibility. Most of the results of this chapter are work by the author and a collaborator, and a couple of technical derivations are placed in the appendix.

# Chapter 1

# Athermality as a quantum resource

We now turn into the detailed description of the resource-theoretic framework from which all the results will build up. It usually goes under the name of *thermal operations*.

The main idea is that we want to define a resource theory that quantifies non-equilibrium, that is, states of systems that are not thermal. This means we want to include processes that drive a system towards its equilibrium state with some environment or bath, and we want to quantify this non-equilibrium and how it is destroyed by the interactions.

Therefore, thermal states will be the *free* elements of the resource theory, those that do not have any value associated to them. We of course also want to include interactions in the theory, but such that we can keep track of all the flows of energy and entropy between the different elements, so the operations that do not generate any resource by themselves will be unitaries that conserve the total energy.

The other ingredient that we will also want to include is the notion of thermodynamical *work*. There are various ways in which this last point can be done. In this section we will only cover the idea of *deterministic* work, whereas at a later stage we will introduce a more refined and general notion of work into the theory.

We start this chapter by defining and explaining in detail the properties of the different elements of the resource theory, and then we will be exploring the first natural questions that come out of it once it is laid out: which transformations of states are possible, and how much work can be extracted or needs to be spent for particular processes to happen.

## 1.1 The ingredients of the resource theory

### 1.1.1 Thermal states: Understanding the heat bath

In many different physical contexts one has a system with some state, in the presence of some environment, which will quite frequently be a very large system in thermal equilibrium. A generic initial state of the system will not be in equilibrium with the bath (that is, in a thermal state), but the joint dynamics will in general drive it towards it. This is the kind of situation we want to describe with this framework, and for that we first need to specify what is the environment (or heat bath) we will be focusing on.

Throughout this section we will assume the bath is of finite size and explore how limiting that is, after which we will describe what advantage does an infinite-size bath give. Let us now define the key properties of the heat bath.

**Definition 1** (Heat bath)**.** *We define a heat bath as a large (but not necessarily infinitely large) system represented by a Hilbert space $\mathcal{H}_{\mathcal{B}}$. It has an effectively continuous number of states given by $\Omega(E, V) = e^{S(E,V)}$, where $S(E, V)$ is the entropy in the microcanonical ensemble for a given energy $E$ and a dimensionless volume $V$ (such as, for instance, the total number of particles). It is such that the following assumptions hold:*

1. *The entropy $S(E, V)$ is extensive: $S(kE, kV) = kS(E, V)$ for all $k > 0$*
2. *The dimensionless volume $V$ is large.*
3. *The bath is in a Gibbs state with a given inverse temperature $\beta$, such that a microstate of energy $E$ has probability $\frac{1}{Z_B}e^{-\beta E}$. This means it is equilibrated with respect to a further, larger bath.*

What is the logic behind this set of assumptions? One should think of this bath as a very large system that is part of an even larger one with an effectively infinite volume with which it is in contact, such that both have been interacting for a long time in the past and are already in thermal equilibrium. The interaction time with the system will be finite, and within such time, a system can only probe such large but finite part of that bath. With this, we are assuming that the interactions within the bath have some sort of light-cone structure, possibly given by some kind of Lieb-Robinson bounds [109], which bound the speed at which information can travel through locally interacting many-body systems. We illustrate this idea in Fig. 1.1.

Assumption 1 implies that we can write the entropy $S(E, V)$ as

$$S(E, V) = V f(u) \tag{1.1}$$

for some function $f(u)$ of the energy density $u = E/V$. The probability distribution for $u$ is then

$$p(u) \propto e^{V[f(u)-\beta u]} \ . \tag{1.2}$$

In the large $V$ limit we can use the saddle point approximation [38]

$$p(u) \propto e^{V\left[f(u_\beta)+\frac{1}{2}f''(u_\beta)(u-u_\beta)^2\right]} \ , \tag{1.3}$$

where $u_\beta$ is the absolute maximum of $f(u) - \beta u$ as a function of $u$, which implies

$$f'(u_\beta) = \beta \ , \tag{1.4}$$

$$f''(u_\beta) < 0 \ . \tag{1.5}$$

In summary, we have a normal distribution

$$p(u) \propto e^{-\frac{V}{2}|f''(u_\beta)|(u-u_\beta)^2} \ , \tag{1.6}$$

with mean $\langle u \rangle = u_\beta$ and variance $\langle (u - \langle u \rangle)^2 \rangle = |V f''(u_\beta)|^{-1}$.

Now, let us relate $f''(u_\beta)$ to the heat capacity, defined as

$$C = V \frac{\mathrm{d}\langle u \rangle}{\mathrm{d}T} = -\frac{V}{T^2} \frac{\mathrm{d}\langle u \rangle}{\mathrm{d}\beta} \ . \tag{1.7}$$

Differentiating Eq. (1.4) with respect to $\beta$ gives $f''(u_\beta)\frac{\mathrm{d}u_\beta}{\mathrm{d}\beta} = 1$, and substituting in Eq. (1.7) gives

$$C = -\frac{V}{T^2} \frac{1}{f''(u_\beta)} \ . \tag{1.8}$$

Note that Eq. (1.5) implies that the heat capacity is positive, as is always the case in "ordinary matter" [1]. Also note that $C \propto V$, because $f(u_\beta)$ is independent of $V$. Which implies that the fluctuations of $u$ are

$$\left\langle (u - \langle u \rangle)^2 \right\rangle^{1/2} = \frac{T\sqrt{C}}{V} \propto V^{-1/2} \ , \tag{1.9}$$

---

[1] Black holes are a notable exception to this rule.

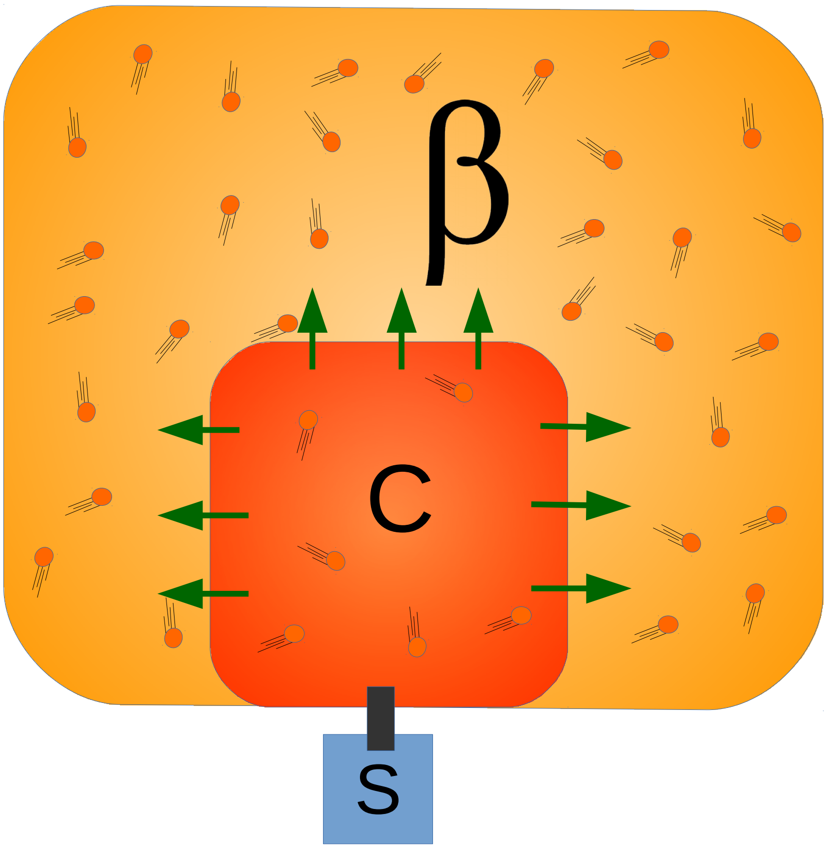

Figure 1.1: We here sketch a very large bath (orange region) of which, given a finite time of interaction, only a finite region of heat capacity $C$ is reached (red region). The system is locally coupled to a part of the finite region. As the time increases and information spreads, this region may get larger, and the infinite-sized approximation becomes more accurate.

which are small when $V$ is large.

Substituting back for $E$, we are finally able to approximate the number of states of the bath as

$$\Omega(E,V) \propto \exp\left(\beta E - \frac{\gamma E^2}{2}\right), \tag{1.10}$$

where we have rescaled the energy such that $\langle E \rangle = 0$, and we define $\gamma = \frac{1}{CT^2}$ as the inverse of the heat capacity.

We will be making the approximation that the energy scales of the system that interact with the bath are small compared to the energy fluctuations of the bath. This is accurate provided the bath is sufficiently large. In particular, we assume that $E_i \ll 1/\sqrt{\gamma}$ for all $E_i$ labelling the energy levels of the system. Effectively this means we can approximate the density of states from Eq. (1.10) as

$$\Omega(E - E_i) \simeq \Omega(E) e^{-(\beta - \gamma E)E_i}. \tag{1.11}$$

We will be using this expression in the coming sections, when analyzing the power of thermal operations.

### 1.1.2 Interactions and conservation of energy

We have a system in some quantum state represented by a density matrix $\rho \in \mathcal{S}(\mathcal{H}_\mathcal{S})$, and with an associated Hamiltonian $H_S$. Our aim is to explore what happens when this system interacts with the heat bath, in such a way that a state which is not at thermal equilibrium will get closer to it. How can we do this from a resource-theoretic perspective? A natural restriction is to impose that the interactions between system and bath are such that the total energy is conserved. If this was not the case, one could attribute a particular change of energy to an external source, which would have to be accounted for as an extra resource.

Perhaps the most obvious example of this kind of interaction is a weak coupling between system and bath. We will focus on the role that this kind of interaction plays within this framework in Chapter 4 but we do not necessarily want to restrict ourselves to it. We only want to be able to keep track of energy, so the interactions we allow for as free operations will be more general.

The Hamiltonian of our system of interest is $H_S$, and the Hamiltonian of the heat bath is $H_B$. A unitary within this resource theory will obey the following property:

**Definition 2** (Energy-conserving unitaries)**.** *An energy conserving unitary $U$ between system and bath (thus acting on the joint Hilbert space $\mathcal{H_S} \otimes \mathcal{H_B}$) is defined as*

$$[U, H_S + H_B] = 0 \tag{1.12}$$

A physical examples of this kind of unitary can be found in Section 1.7. For now, we can take this as the defining property of the set of free operations of the resource theory, which again we will refer to as *thermal operations*.

**Definition 3** (Thermal operations)**.** *A particular quantum map $T(\cdot)$ on a system $S$ is a thermal operation if and only if it can be written as*

$$T(\rho) = \mathrm{Tr}_B[U(\rho \otimes \tau_\beta)U^\dagger], \tag{1.13}$$

*where $U$ is an energy-conversing unitary, and*

$$\tau_\beta = \frac{e^{-\beta H_B}}{Z_B} \tag{1.14}$$

*represents the thermal state of the bath with Hamiltonian $H_B$, inverse temperature $\beta$ and partition function $Z_B = e^{-\beta H_B}$.*

From these definitions, we straightforwardly obtain the following Lemma.

**Lemma 1.** *Let $T(\cdot)$ be a thermal operation between a system and a bath at inverse temperature $\beta$, and let us define the thermal state of the system $S$ with Hamiltonian $H_S$ as*

$$\tau_S = \frac{e^{-\beta H_S}}{Z_S}, \tag{1.15}$$

*where $Z_S = \mathrm{Tr}[e^{-\beta H_S}]$ is the partition function of the system. The thermal state of the system is left invariant*

$$T(\tau_S) = \tau_S. \tag{1.16}$$

*Proof.* It follows straightforwardly from the fact that the unitary is constrained to be energy-conserving:

$$\begin{aligned} T(\tau_S) &= \mathrm{Tr}_B[U\tau_S \otimes \tau_\beta U^\dagger] \\ &= \mathrm{Tr}_B[\tau_S \otimes \tau_\beta] \\ &= \tau_S. \end{aligned} \tag{1.17}$$

Here to go from the first to the second line we have used the fact that $[U, H_S + H_B]$, which implies that $[U, \tau_S \otimes \tau_\beta]$. □

The following property of thermal operations will also be of importance. It was first noticed in this form in [115].

**Lemma 2.** *[Time-translation invariance] Let us define the unitary quantum channel on the Hilbert space of the system $S$ representing* time translation *as*

$$\mathcal{G_S}^t(\cdot) = e^{-iH_S t}(\cdot)e^{iH_S t}. \tag{1.18}$$

*Take a thermal operation applied to a system with a Hamiltonian $H_S$. The action of a thermal operation commutes with these time translations*

$$T(\mathcal{G_S}^t(\cdot)) = \mathcal{G_S}^t(T(\cdot)). \tag{1.19}$$

*Proof.* We need to use the energy-conservation property of the unitary, and the fact that the bath is initially in a stationary state with respect to its Hamiltonian $H_B$. Let us write

$$T(\mathcal{G_S}^t(\rho)) = \mathrm{Tr}_B[Ue^{-iH_S t}(\rho)e^{iH_S t} \otimes \tau_\beta U^\dagger] \tag{1.20}$$

$$= \mathrm{Tr}_B[Ue^{-iH_S t}(\rho)e^{iH_S t} \otimes e^{-iH_B t}(\tau_\beta)e^{iH_B t}\tau_\beta U^\dagger] \tag{1.21}$$

$$= \mathrm{Tr}_B[Ue^{-i(H_S+H_B)t}(\rho \otimes \tau_\beta)e^{i(H_S+H_B)t}U^\dagger] \tag{1.22}$$

$$= \mathrm{Tr}_B[e^{-i(H_S+H_B)t}U(\rho \otimes \tau_\beta)U^\dagger e^{i(H_S+H_B)t}] \tag{1.23}$$

$$= \mathcal{G_S}^t(T(\cdot)) \tag{1.24}$$

□

This property has some important implications for the action of thermal operations on states. In particular, we proceed to show that it allows us to restrict ourselves to the set of quantum states that do not have coherences in the energy eigenbasis, which are significantly easier to deal with. The problem of dealing with coherence in this approach to quantum thermodynamics is a very important one, but fewer results exist regarding which transitions between states are possible. We outline some of the most important ones in Section 1.6.

In any case, most of the work presented here will focus on that subset of states that do not have coherence in the energy eigenbasis. These are defined as

**Definition 4** (Quasiclassical states)**.** *A quantum state $\rho$ is* quasiclassical *if and only if* $[\rho, H_S] = 0$.

We now define the following operation

**Definition 5.** *[Decoherence in energy] We define the following decoherence map*

$$\Delta_S(\rho) = \lim_{T\to\infty} \frac{1}{T}\int_{-T}^{T} \mathcal{G_S}^t(\rho)\,dt = \lim_{T\to\infty} \frac{1}{T}\int_{-T}^{T} e^{-iH_St}(\rho)e^{iH_St}\,dt. \tag{1.25}$$

The fact that $\lim_{T\to\infty}\frac{1}{T}\int_{-T}^{T} e^{-i\omega t}\mathrm{d}t = 0$ for $\omega \neq 0$ means that all the rotating terms in the density matrix $e^{-iH_St}(\rho)e^{iH_St}$ vanish. From this one can see that this map destroys all the coherence of a quantum state in the eigenbasis of $H_S$, except for that which is within degenerate subspaces of energy. That is, $\Delta_S(\rho)$ is always a quasiclassical state, independently of $\rho$. Through this definition, one can see that an equivalent way of characterizing quasiclassical states is that they are invariant under decoherence, such that $\Delta_S(\rho) = \rho$.

What happens when there are degeneracies in the energy spectrum? In that case the state $\Delta_S(\rho)$ may have some coherence within that degenerate subspace, but we can use an energy-conserving unitary $U_S$ (a free operation) on the system alone to rotate that subspace into its diagonal form. As an example, for two degenerate levels with labels $k$ and $k+1$, we can freely rotate

$$U_S \begin{pmatrix} p_1 & ... & ... & 0 \\ ... & \rho_{k,k} & \rho_{k,k+1} & ... \\ ... & \rho_{k+1,k} & \rho_{k+1,k+1} & ... \\ 0 & ... & ... & p_n \end{pmatrix} U_S^\dagger = \begin{pmatrix} p_1 & ... & ... & 0 \\ ... & p_k & 0 & ... \\ ... & 0 & p_{k+1} & ... \\ 0 & ... & ... & p_n \end{pmatrix}. \tag{1.26}$$

Therefore, we can always take a state with coherence in degenerate subspaces to be a diagonal state. Given a particular choice of eigenvectors of $H_S = \sum_{i=1}^{n} E_i |E_i\rangle\langle E_i|$, where the index $i$ runs over the $n$ different eigenvectors, we can hence always write a quasiclassical state $\Delta_S(\rho)$ in terms of that eigenbasis as

$$\Delta_S(\rho) = \sum_i p_i |E_i\rangle\langle E_i|, \tag{1.27}$$

where $p_i$ is a probability distribution where each element is a particular energy eigenstate, and hence represents the *populations* of state $\rho$.

We finally arrive to the central result of the section.

**Theorem 1.** *Let us take a thermal operation $T(\cdot)$ and an initial quasiclassical state $\rho = \sum_i p_i |E_i\rangle\langle E_i|$. The state $\sigma = T(\rho)$ is also a quasiclassical state $\sigma = \sum_{j=1}^{n} q_j |E_j\rangle\langle E_j|$ and the initial and final populations are related by*

$$q_j = \sum_{i=1}^{n} P(j|i) p_i, \tag{1.28}$$

*where $P(j|i) = \langle E_j | T(|E_i\rangle\langle E_i|) | E_j\rangle$ is a $n \times n$ stochastic matrix with the following properties*

1. *$P(j|i) \geq 0 \;\forall\, i, j$ (positivity)*
2. *$\sum_{j=1}^{n} P(j|i) = 1 \;\forall\, i$ (stochasticity)*
3. *$\sum_{i=1}^{n} P(j|i) \frac{e^{-\beta E_i}}{Z_S} = \frac{e^{-\beta E_j}}{Z_S} \;\forall\, j$ (preservation of the Gibbs distribution)*

*Proof.* By using Lemma 2 and Definition 5 we can see that

$$T(\Delta_S(\cdot)) = \Delta_S(T(\cdot)), \tag{1.29}$$

that is, the decoherence map commutes with the action of a thermal operation. This directly implies that if the input of a thermal operation is quasiclassical $\rho = \Delta_S(\rho)$, then so is the output, as

$$\sigma = T(\rho) = T\Delta_S(\rho) = \Delta_S(T(\rho)) = \Delta_S(\sigma). \tag{1.30}$$

We can then write $\sigma = \sum_{j=1}^{n} q_j |E_j\rangle\langle E_j|$ for some probability distribution $q_j$. Now to get to Eq. (1.28) we write

$$q_j = \langle E_j|\sigma|E_j\rangle = \langle E_j|T(\sum_{i=1}^{n} p_i |E_i\rangle\langle E_i|)|E_j\rangle \tag{1.31}$$

$$= \sum_{i=1}^{n} \langle E_j|T(|E_i\rangle\langle E_i|)|E_j\rangle p_i = \sum_{i=1}^{n} P(j|i)p_i. \tag{1.32}$$

After this, the positivity property follows from the fact that the quantum map $T(\cdot)$ is positive. The stochasticity property follows from the fact that it is trace-preserving, and the property of preserving the Gibbs distribution is a rewriting of Lemma 1.

□

This theorem has an important implication: the action of thermal operations on quasi-classical states is equivalent to the action of a stochastic matrix on the populations, with the condition that that stochastic matrix preserves the thermal distribution of the system.

### 1.1.3 Work storage

If we understand systems out of equilibrium as resources, what is it that they can be used for? The most obvious task is that of extracting work, or useful energy. The way we will be modelling this thermodynamical work is via introducing an additional system into our setting, a work storage device or *battery* that absorbs or supplies the energy that we will be referring to as work.

In Chapter 3 we will be further exploring different possible definitions of work. For now, and for simplicity and consistency of presentation, we will be talking about work only as the more restricted notion of *deterministic work*, first introduced in [89].

Let us take a battery, which is a system with a Hamiltonian $H_W$ defined as

$$H_W = (W + E_0)|W\rangle\langle W| + E_0|0\rangle\langle 0|, \tag{1.33}$$

where $|W\rangle\langle W|$ represents an excited state, $|0\rangle\langle 0|$ is the ground state if $W > 0$ and the excited state otherwise, and one can always choose $E_0 = 0$. We will be assuming that whenever we want to extract an amount of work given by $W$, we are able to bring in to our thermodynamic protocol a battery with that gap.

Effectively what happens in this context is that we will be looking at the interaction of the bath with the system and battery together as if they were a new effective system, with a joint Hamiltonian $H_{SW} = H_S + H_W$ (note that each of the two terms has a nontrivial action in one of the two subsystems only). We will hence assume energy conservation between system, bath and battery, so that Eq. (1.39) transforms into

$$[U, H_S + H_W + H_B] = 0. \tag{1.34}$$

We will then be focusing on transitions such as

$$\rho \otimes |W\rangle\langle W| \xrightarrow{\text{TO}} \sigma \otimes |0\rangle\langle 0| \tag{1.35}$$

in which work $W$ is spent, and

$$\rho \otimes |0\rangle\langle 0| \xrightarrow{\text{TO}} \sigma \otimes |W\rangle\langle W| \tag{1.36}$$

in which work $W$ is stored, or $-W$ is spent. Thus we can also understand $W$ also as a negative quantity.

We are interested in which of these transitions can be realized through the application of thermal operations, as indicated by the symbol "$\xrightarrow{\text{TO}}$". It will be useful to define the following quantity:

**Definition 6.** *[Work of transition] Given any two quasiclassical states $\rho$ and $\sigma$, the work of transition $W_{\rho\longrightarrow\sigma}$ is defined as*

- *When $\rho \overset{TO}{\to} \sigma$ is a possible transformation: the largest possible $W$ such that the transition*

$$\rho \otimes |0\rangle\langle 0| \xrightarrow{TO} \sigma \otimes |W\rangle\langle W| \tag{1.37}$$

  *is possible, in which case $W_{\rho\to\sigma} \geq 0$.*

- *Otherwise, when the transition is not possible without the assistance of work, it is defined as the minimum $W$ such that the transition*

$$\rho \otimes ||W|\rangle\langle |W|| \xrightarrow{TO} \sigma \otimes |0\rangle\langle 0| \tag{1.38}$$

  *is possible, in which case $W_{\rho\to\sigma} \leq 0$.*

In this definition we care about the "largest possible" value of $W$ because lower values of $W$ than that maximum can also be extracted along a transition of the form of Eq. (1.37), and thus the maximum is the one value that gives the relevant information about what values of the work are possible. An analogous reasoning applies for the case of negative work in (1.38).

Two special cases of this notion will be particularly important, which are the work of transition when either the final or the initial states are thermal.

**Definition 7.** *[Extractable work] The extractable work from a state* $\rho$ *is defined as* $W_{\mathrm{e}}(\rho) = W_{\rho\to\tau_S}$.

**Definition 8.** *[Work of formation] The work of formation from a state* $\rho$ *is defined as* $W_f(\rho) = -W_{\tau_S\to\rho}$.

The thermal state is the only non-resourceful state, as for any given state $\rho$ there always exists a thermal operation such that $T(\rho) = \tau_S$ (this will become apparent in the next sections). This implies that $W_{\mathrm{e}}(\rho) \geq 0$, as any state can be brought to the thermal state without expending any work. Analogously, Lemma 1 implies that $W_{\mathrm{f}}(\rho) \geq 0$, as one cannot create a non-thermal state without spending work.

## 1.2 Towards thermomajorization

In this section we proceed to answer a central question of the resource theory: given a state $\rho$, what is the set of target states $\sigma$ that can be accessed via the set of thermal operations?

We shall first describe what is the power of thermal operations with a finite bath when no work is involved, and only system-bath interactions occur. After that, we will be able to consider deterministic work extraction and expenditure using the same tools, by considering the battery as part of our system. We will be focusing on the case of quasiclassical states, and later briefly describe what is known for more general states.

For the sake of presentation, let us first focus on the case of a finite bath, for which in general no definite conclusions can be given, and we will later take the limit of an infinite bath, where the situation simplifies dramatically.

We recall the property of energy conservation of the unitaries

$$[U, H_S + H_B] = 0, \tag{1.39}$$

as the battery is not involved for now.

We now append a system with a Hamiltonian $H_S = \sum_i E_i |E_i\rangle\langle E_i|$ and quasiclassical state $\rho = \sum_i p_i |E_i\rangle\langle E_i|$ to the finite bath, such that they are in an initially uncorrelated state $\rho \otimes \tau_\beta$. Because of the form of Eq. (1.39), we want to look at subspaces of fixed total energy of $\rho \otimes \tau_\beta$, as the dynamics of each such subspace is independent from the rest. Let $\Pi_{E_{\text{tot}}}$ be a projector into a total energy subspace of energy $E_{\text{tot}}$. Any restriction of the state to a subspace can be written as

$$\begin{aligned} &\Pi_{E_{\text{tot}}} \rho \otimes \tau_\beta \Pi_{E_{\text{tot}}} = \\ &k_{E_{\text{tot}}} \sum_{i=1}^{n} \sum_{b \in \mathcal{M}(E_{\text{tot}} - E_i)} p_i e^{\beta(E_i - E_{\text{tot}})} |E_i\rangle\langle E_i| \otimes |b\rangle\langle b|, \end{aligned} \tag{1.40}$$

where $k_{E_{\text{tot}}}$ is a normalization constant, and $\mathcal{M}(E)$ is the set of eigenstates of the bath with energy $E$, which has cardinality $\Omega(E)$ (the number of states of the bath).

Because we are assuming the bath is thermal, and the state of the system is quasiclassical, we have that

$$\rho \otimes \tau_\beta = \sum_{E_{\text{tot}}} \Pi_{E_{\text{tot}}} \rho \otimes \tau_\beta \Pi_{E_{\text{tot}}}. \tag{1.41}$$

Invoking the approximation that leads to Eq. (1.10), we can write

$$\Omega(E_{\text{tot}} - E_i) \simeq \Omega(E_{\text{tot}}) e^{-(\beta - \gamma E_{\text{tot}}) E_i}. \tag{1.42}$$

This gives the size of the subspace with the same $E_{\text{tot}}, E_i$ that appears in the expansion of Eq. (1.40). In each of these subspaces the projectors have weights $\propto k_{E_{\text{tot}}} e^{-\beta E_{\text{tot}}} p_i e^{\beta E_i}$.

We shall now define the following concept, which will be very useful in the rest of the chapter.

**Definition 9** ($\beta$-order)**.** *Let us take a quasiclassical state with populations $p_i$. The $\beta$-order is a relabelling of the i-th index labelling the energy eigenstates $E_i$ such that*

$$p_1 e^{\beta E_1} \geq p_2 e^{\beta E_2} \geq .... \geq p_n e^{\beta E_n}. \tag{1.43}$$

Now, for any given joint state $\rho$, this ordering allows us to draw a so-called *majorization histogram* for the subspace of fixed total energy. An illustration of how this is constructed is shown in Fig. 1.2. This majorization histogram represents all the microstates of a particular subspace of total energy, and the height of each of the bars is proportional to $p_i e^{\beta E_i}$, so that the $\beta$-order guarantees that the height of the bars decreases along the diagram.

We can now look at the effect of an arbitrary energy-conserving unitary $U$ to the joint system-bath pair. The constraint of energy conservation implies that the unitary can be written as (see Appendix C of [89])

$$U = \bigoplus_{E_{\text{tot}}} U_{E_{\text{tot}}}, \tag{1.44}$$

where the direct sum is over all different subspaces of fixed total energy, and $U_{E_{\text{tot}}}$ is an arbitrary unitary acting only on a subspace of fixed total energy. We shall assume that there is an extra resource we can bring in from the bath: a source of randomness we can condition on, such that we not only can apply an energy-conserving unitary, but also a convex mixture of them, such as

$$(\cdot) \longrightarrow \sum_{\lambda} p_\lambda U_\lambda (\cdot) U_\lambda^\dagger, \tag{1.45}$$

for some set of energy conserving unitaries $U_\lambda$ and any probability distribution over that set $p_\lambda$.

We arrive to the following conclusion, which we phrase as an observation.

**Observation 1.** *The set of mixtures of energy-conserving unitaries is equivalent to the set of mixtures of independent, arbitrary unitaries on separate subspaces of fixed system-bath total energy.*

As an example, let us take a unitary of the form of (1.44) which is such that each $U_{E_{\text{tot}}}$ permutes the energy eigenstates of each subspace in some way. Given that a permutation is a bijection, this operation is reversible (just apply the inverse permutation). Another allowed unitary may for instance be the identity matrix, which has a trivial effect. We can thus think of an operation which with probability $p$ applies the first permutation and with probability $1-p$ applies the identity operator. Now, this probabilistic mixture of bijections is not a bijection itself. The induced map on system-bath, even if it is composed of reversible operations, will be irreversible. These irreversible maps are what we are allowing for in this resource theory.

The next step is the definition of the very important concept of majorization:

**Definition 10** (Majorization). *Given two probability distributions $\lambda(s)$ and $\eta(s)$ with $n$ elements, ordered such that $\lambda(s+1) \geq \lambda(s)$ and $\eta(s+1) \geq \eta(s)$, we say $\lambda(s)$ majorizes $\eta(s)$ if it is true that*

$$\sum_{s=1}^{k} \lambda(s) \geq \sum_{s=1}^{k} \eta(s) \ \ \forall k \in \{1, ..., n\}. \tag{1.46}$$

Now we invoke the following theorem. For a complete proof, we refer the reader to Appendix A of [80].

**Theorem 2.** *The spectrum of an arbitrary quantum state $\rho$ majorizes that of a state $\sigma$ if and only if there exists a probability distribution $p_\lambda$ and a set of unitaries $U_\lambda$ such that*

$$\sigma = \sum_{\lambda} p_\lambda U_\lambda(\rho) U_\lambda^\dagger. \tag{1.47}$$

To prove the “only if” this theorem, one needs to use the fact that a mixture of unitaries is a unital map, that preserves the identity matrix. This means that its effect on the spectra of the input state is that of a doubly stochastic matrix (that is, one that preserves the uniform distribution). The “if” direction can be proved by explicitly constructing a mixture of unitaries.

This is an important theorem that implies that the probability spectrum of $\sigma$ is more uniform than that of $\rho$. This notion of “non-uniformity” is captured in the definition of majorization, which is a quasi-ordering of the states, in which the “noisier” or “more uniform” states are majorized by the less uniform or less noisy ones. The fact that the spectrum of the output $\sigma$ is noisier can be thought of as a consequence of the mixture of unitaries being an irreversible map, and not a bijection for which a mathematical inverse exists.

Essentially here we apply this theorem by taking as an input state $\rho$ the subnormalized state

$$\Pi_{E_{\text{tot}}} \rho \otimes \tau_\beta \Pi_{E_{\text{tot}}}, \tag{1.48}$$

for a given total energy $E_{\text{tot}}$ (if we want a normalized state, we just have to divide by the probability of such a total energy). As a target state, we choose equivalently the subnormalized state

$$\Pi_{E_{\text{tot}}} \sigma \otimes \tau_\beta \Pi_{E_{\text{tot}}}. \tag{1.49}$$

With this choice, Theorem 2 implies here that, within a subspace of total energy, the set of states that can be reached using thermal operations is that for which the majorization criteria between the spectra holds (that is, the spectra of the initial majorizes that of the final one).

Putting everything together, we arrive to the central statement of this section:

**Lemma 3.** *A transition between two different states of system and bath of the form $\rho\otimes\tau_\beta$ and $\sigma\otimes\tau_\beta$ is possible under thermal operations if and only if in each of the total energies $E$ the probability spectrum of $\rho\otimes\tau_\beta$, as seen in the majorization histogram (an example of which is Fig. 1.2), majorizes that of $\sigma\otimes\tau_\beta$.*

*Proof.* In order to show this we just need to combine the statements of Theorem 2 and Observation 1: the effect of thermal operations is that of combinations of arbitrary unitaries in definite energy subspaces, and hence we can apply Theorem 2 to each of these subspaces separately. □

The statement of this Lemma is perhaps more clearly expressed in terms of *thermomajorization diagrams.* We may define the concave 2D diagram, with origin at $(0,0)$, as the curve resulting from consecutively joining the points given by

$$\Big\{\Big(\sum_{i=1}^{k} e^{-(\beta-\gamma E_{\text{tot}})E_i}, \frac{\sum_{i=1}^{k} p_i e^{\gamma E_{\text{tot}} E_i}}{\sum_{i=1}^{n} p_i e^{\gamma E_{\text{tot}} E_i}}\Big)\Big\} \;\forall k\in\{1,...,n\} \tag{1.50}$$

where the eigenstates are labeled according to the $\beta$-ordering. Each segment of this diagram corresponds to a particular energy eigenstate of the system, and is constructed by subsequently adding the probability weight of each of the individual "microstates" of the majorization histogram (the individual bars of Fig. 1.2).

Majorization of one state by another within a particular subspace of total energy $E_{\text{tot}}$ is then equivalent to the inital thermomajorization diagram of energy $E_{\text{tot}}$ lying strictly above that of the target one. When this happens, we say that the initial state thermomajorizes the final for a given energy $E_{\text{tot}}$. Hence, we have that for each energy $E_{\text{tot}}$ there is a slightly different thermomajorization-like criteria, and for a transition to be possible with complete certainty all of them apply. An example of such a diagram is given in Fig. 1.3.

Each diagram is given by a particular energy, and to give a conclusive answer we have to check within the whole range of possible $E_{\text{tot}}$, which may not be feasible in general, as the range of $E_{\text{tot}}$ is effectively continuous.

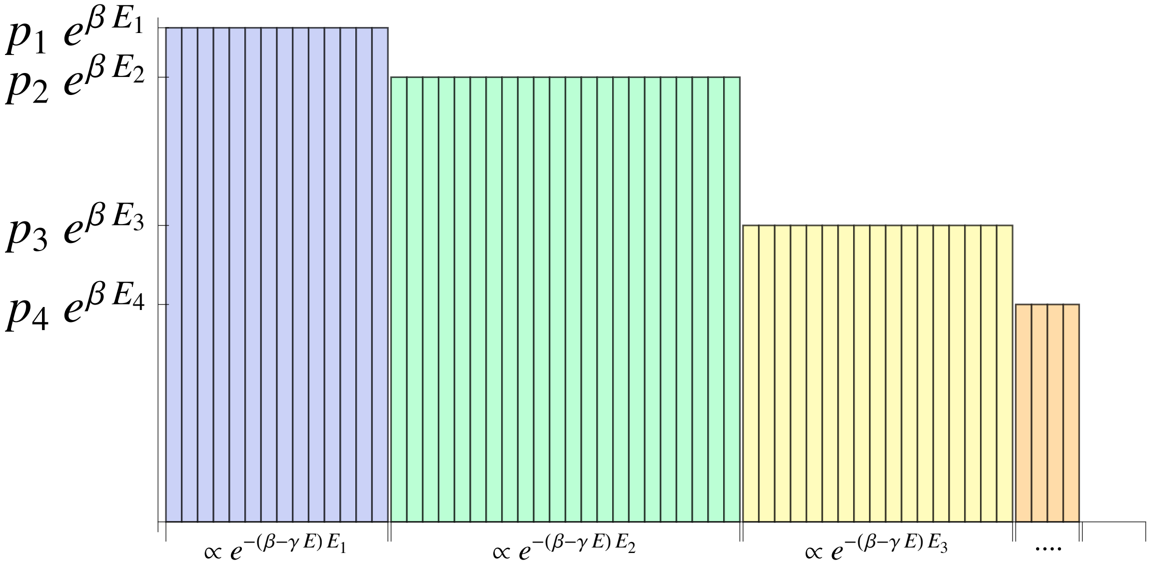

Figure 1.2: We show the majorization histogram of a particular subspace of total energy $E$ of the joint system-bath product state, where the system is in state $\rho = \sum_i p_i |E_i\rangle\langle E_i|$ diagonal in energy, and with the energy levels $\beta$-ordered such that $p_k e^{\beta E_k} \geq p_{k+1} e^{\beta E_{k+1}}$. The parameter $\gamma$ is related to the heat capacity of the bath as $\gamma = \frac{1}{CT^2}$. From the fact that the height of the individual bars is $p_i e^{\beta E_i}$ we can see that the thermal distribution corresponds to the case of the whole diagram being flat.

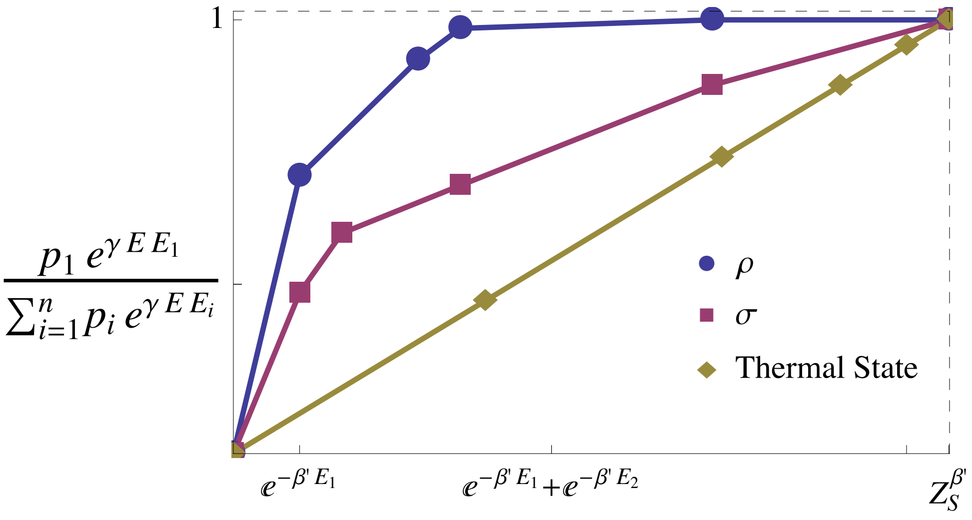

Figure 1.3: We show an example of a thermomajorization diagram for three different states of a 3-level system, $\rho$, $\sigma$ and the thermal state, at a point with a total energy of $E$ (and where $\beta' = \beta - \gamma E$). The $\beta$-order in each of the curves is different, and at this particular total energy the transitions $\rho \rightarrow \sigma$ is possible, as the diagram of $\rho$ lies above that of $\sigma$. Here $Z_S^{\beta'} = \sum_i e^{-\beta' E_i}$.

In any case, considering the full range of total energies may not be necessary in particular cases. The probability distribution of total energies is approximately a Gaussian with tails that cause the range of energies we have to check to be very large. However, the further a particular total energy is from the mean, the less likely it is to occur. Hence, this criteria may give a definite answer if we are willing to omit the tails of the distribution of energy of the bath, and just consider a certain range of total energies. In that case, if we obtain an answer such as "the transition $\rho \overset{TO}{\to} \sigma$ is possible", we can be confident, with probability $1-\epsilon$, that this answer will be correct. The next subsection is devoted to analyzing the tradeoff between the range of energies that need to be checked and the probability of failure.

### 1.2.1 Total energy distribution

Given that we have the energy distributions of both bath and system, we can obtain the total energy distribution.

$$p(E_{\mathrm{tot}}) \propto \sum_{i=1}^{n} e^{-\frac{\gamma}{2}(E_{tot}^2 - E_{tot}E_i)} p_i, \tag{1.51}$$

which is a convex mixture of Gaussians with width $1/\sqrt{\gamma}$, each with its centre offset by $E_i$. By taking again the approximation of Eq. (1.11) above, that $1/\sqrt{\gamma} \ll E_i$, the total energy distribution is then very close to that of just the bath, so $E_{\mathrm{tot}} \sim E \sim \gamma^{-1/2}$ and

$$p(E_{\mathrm{tot}}) \approx p_b(E) \propto e^{-\frac{\gamma}{2}E^2}. \tag{1.52}$$

Now say we do not necessarily want a conclusive answer from the thermomajorization criteria, but only one that we can be confident about with a very high probability $1-\epsilon$. In that case, we may only have to check the criteria for a range of energies $\{E_{\min}, ..., E_{\max}\}$, where the relation between this range and the probability $\epsilon$ is given by

$$1 - \epsilon = \int_{E_{\min}}^{E_{\max}} \sqrt{\frac{\gamma}{2\pi}} e^{-\frac{\gamma}{2}E^2} \mathrm{d}E. \tag{1.53}$$

We may define two minimum and maximum effective temperatures given by

$$\beta_{+} = \beta - \gamma E_{\max} \tag{1.54}$$

$$\beta_{-} = \beta - \gamma E_{\min}. \tag{1.55}$$

If we take $-E_{\min} = E_{\max} = E^*$, then

$$\epsilon = 2\sqrt{\frac{\gamma}{\pi}} \int_{E^*}^{\infty} e^{-\gamma E^2} \mathrm{d}E. \tag{1.56}$$

For large $x$ we can approximate this error function as

$$\operatorname{errf}(x) = \frac{1}{\sqrt{\pi}} \int_{-x}^{x} e^{-t^2} \mathrm{d}t \simeq 1 - \frac{e^{-x^2}}{\sqrt{\pi} x}. \tag{1.57}$$

Hence we can approximate

$$\epsilon \simeq 2^{3/2} \frac{e^{-\frac{\gamma}{2} E^{*2}}}{\sqrt{\pi\gamma} E^*} \tag{1.58}$$

This expression gives the tradeoff between the range of thermomajorization diagrams we need to check, which will be $E \in \{-E^*, ..., E^*\}$, and the probability that the conclusion given by the thermomajorization diagrams is not valid.

What does this mean? What we want to show with this is that, even if the range of total energies is very large, one can restrict to a much narrower range around the average, and be confident that the criteria will only give the wrong answer with a very low probability. Effectively, this means we only have to check thermomajorization diagrams within a finite range. This still implies a very large amount of diagrams, which again may not be a feasible procedure in practice.

We however want to illustrate this for two reasons that will become clear in later sections: *i)* we do not have to check all the diagrams for particular transitions, and *ii)* all the diagrams collapse to the same one in the limit of an infinite heat bath.

### 1.2.2 Fully degenerate energy spectrum

Before ending this section, it is worth pointing out a particularly simple case that will be useful later: that of fully degenerate Hamiltonians, where $H_S = c\mathbb{I}$ for some constant $c$, and hence all the energy levels are the same. In that case, the thermomajorization diagram is made out of the following set of points

$$\Big\{ \Big( \sum_{i=1}^{k} e^{-(\beta - \gamma E_{\mathrm{tot}})c}, \frac{\sum_{i=1}^{k} p_i}{\sum_{i=1}^{n} p_i} \Big) \Big\} \ \forall k \in \{1, ..., n\}. \tag{1.59}$$

We see then that the only input to this diagram is the probability spectrum, as the sum $\sum_i^k e^{-(\beta - \gamma E_{\mathrm{tot}})c}$ is just a sum over constant terms and hence the particular values of $\beta, \gamma, E_{\mathrm{tot}}$

and $c$ do not play a role in whether a probability distribution majorizes another one or not. Therefore, in this case, a state thermomajorizes another if and only if the former also majorizes the latter:

**Lemma 4.** *Let us take the particular case of a system with a degenerate Hamiltonian* $H \propto \mathbb{I}$*. In that case,* $\rho \xrightarrow{TO} \sigma$ *is possible if and only if the spectrum of* $\rho$ *majorizes that of* $\sigma$*.*

*Proof.* By inspection, the horizontal axis of the thermomajorization diagram is split into segments of equal length. This means the $\beta$-order is now just an order given by the magnitude of the probabilities as $p_1 \geq p_2 \geq ... \geq p_n$, and one curve is above the other if and only if one probability distribution majorizes the other, as given by Definition 10. ☐

We will be using this fact in Section 2.1, when we introduce a further resource theory: that of noisy operations, where energy does not play a role and only the purity of the states matters.

## 1.3 Deterministic work extraction/expenditure

We are now in a position to calculate the deterministic work in certain transitions, which we can write down explicitly when we allow for a finite probability $\epsilon$ of the thermomajorization criteria not giving the right answer. We specialize to two important cases where the answer can be written in a closed form: extracting work in a transition to a thermal state (as the least resourceful state), and creating an arbitrary state out of a thermal state, as they are the simplest examples.

### 1.3.1 Work extraction in total energy subspaces

From a given initial state $\rho$ we want to extract some deterministic work $W$ given some total energy subspace $E$. Recalling Definition 7, this is equivalent to computing what is the maximum $W$ for which the transition

$$\rho \otimes |0\rangle\langle 0| \rightarrow \tau_S \otimes |W\rangle\langle W|, \tag{1.60}$$

is possible for a given total energy $E$. If a particular value $W$ is possible, then any other lower value of it is possible too (as one can just lower the battery for free). Again, $\tau_S = e^{-\beta H_S}/Z_S$ is the thermal state of the system, and the second part of the tensor product corresponds to the weight. Regarding the maximum possible work, we have the following result.

**Theorem 3.** *The optimal deterministic extractable work that can be extracted from a state $\rho$ using a bath with heat capacity $C$ is*

$$W_e(\rho) = F^{\beta_-}_{min}(\rho), \tag{1.61}$$

*with a probability of the extraction not being possible given by $\epsilon$ defined in Eq.* (1.53) *(in which $\beta_-$ depends on $\epsilon$). The* min*-free energy is defined as*

$$F^{\beta}_{min}(\rho) = \frac{1}{\beta}\log Z_S - \frac{1}{\beta}\log\Big(\sum_{i=1}^{n} e^{-\beta E_i} p_i^0\Big), \tag{1.62}$$

*where we define $p_i^0$ as $1$ if $p_i > 0$ and $0$ otherwise.*

*Proof.* The thermomajorization curve of the final state of Eq. (1.60) is just a straight line, with slope given by $e^{-\beta W}/Z_S$. Hence, in order to check whether the transition is possible we just need to compare the ranks (or the points at which the thermomajorization diagrams reach 1 in the vertical axis) of the subspace of energy $E$ of the states $\rho\otimes|0\rangle\langle 0|\otimes\tau_\beta$ with $\tau\otimes|W\rangle\langle W|\otimes\tau_\beta$. The former is

$$d_{\text{in}} = \sum_{i=1}^{n} \Omega(E-E_i)p_i^0 \simeq \Omega(E)\sum_{i=1}^{n} e^{-(\beta-\gamma E)E_i} p_i^0, \tag{1.63}$$

and the latter is

$$d_{\text{fin}} = \sum_{i=1}^{n} \Omega(E-E_i-W) \simeq \Omega(E)e^{-(\beta-\gamma E)W}\sum_{i=1}^{n} e^{-(\beta-\gamma E)E_i}, \tag{1.64}$$

where we have approximated the densities of states the same way as in Eq. (1.11). In general, we will have that $d_{\text{in}} \leq d_{\text{fin}}$, and both ranks will be equal in the optimal situation where the maximum work $W$ is extracted. Equating and solving for $W$ yields

$$W = F^{\beta'}_{\text{min}}(\rho), \tag{1.65}$$

where $\beta' = \beta - \gamma E$. This, as will be seen in Section 1.4.1 below, is just the 0-order Renyi free energy (as defined in [89]) but with an effective temperature $\beta'$ that fluctuates, depending on the particular value of the total energy $E$ .

The quantity of Eq. (1.65) is the maximum amount of work one can extract for a given energy $E$. If we want to extract truly deterministic work, the work extracted must however be the same independently of what is the actual total energy. The minimum possible $W$ over all $E$ hence gives the highest possible one that can be the same for all energies. The function $\frac{1}{\beta'}F^{\beta'}_{\text{min}}(\sigma)$ is monotonically increasing in $E$, so the minimum is achieved at our chosen $E = E_{\text{min}}$, or in $\beta' = \beta_-$ as defined in Eq. (1.55). This completes the proof.

□

We would like to stress that the probability of error $\epsilon$ does not represent the probability of failing at extracting the work $W$ after a particular $TO$ has been applied. It represents our confidence on the thermomajorization criteria being correct. If the criteria in fact says that there exists a TO that extracts an amount of work $W$, we have to accept that this answer may not be correct, with probability $\epsilon$.

### 1.3.2 Work of formation in total energy subspaces

Now, for a given total energy $E$, we want to find the lowest $W$ for which the transition

$$\tau \otimes |W\rangle\langle W| \to \rho \otimes |0\rangle\langle 0| \tag{1.66}$$

is possible. We again express this with the following result.

**Theorem 4.** *Up to an error probability of $\epsilon$, the minimum deterministic work we need to create a quasi-classical state $\rho$ starting with the thermal state is*

$$W_{for} = \frac{1}{\beta_+}(\log \frac{Z_{\beta_+}}{Z_\beta} + \beta F^{\beta}_{\text{max}}(\rho) + \log \frac{1}{\sum_{i=1}^n p_i e^{\gamma E_{max} E_i}}), \tag{1.67}$$

*where the* max-*free energy is defined as*

$$F^{\beta}_{\text{max}}(\rho) = \frac{1}{\beta} \log \max_i (p_i e^{\beta E_i}), \tag{1.68}$$

*Proof.* Because the curve of the initial state is straight, as it is a thermal state with a battery state tensored in, we only need its slope to be equal to the slope of the first segment (the one corresponding to $E_1$ when $\beta$-ordered) of the final one [89, 75]. This way, we are guaranteed that the thermal+battery state curve is above that of the target state we want to reach, in which case the transition is possible. The slope of the initial state is

$$\frac{e^{\beta' W}}{Z_{\beta'}}, \tag{1.69}$$

and the slope of the initial segment of the final state (and thus the highest, by te convexity of the curve) is

$$\frac{1}{\sum_{l=1}^{n} p_l e^{\gamma E E_l}} \max_i p_i e^{\beta E_i}. \tag{1.70}$$

The smallest possible value of the work will be that in which these two slopes are equal. Thus, equating them and solving for $W$ yields

$$W = \frac{1}{\beta'}(\log\left(Z_{\beta'} \max_i [p_i e^{\beta E_i}]\right) + \log \frac{1}{\sum_{i=1}^{n} p_i e^{\gamma E E_i}}). \tag{1.71}$$

We can decompose this in three terms:

$$W = \frac{1}{\beta'}(\log \frac{Z_{\beta'}}{Z_\beta} + \beta F_{\max}^{\beta}(\rho) + \log \frac{1}{\sum_{i=1}^{n} p_i e^{\gamma E E_i}}). \tag{1.72}$$

In analogy with the extractable work, if we want to create a state with deterministic work we need to find the maximum of these over $E$. The work $W$ in Eq. (1.72) is also monotonically increasing in $E$, and hence the maximum is achieved at $E = E_{\max}$, or equivalently in $\beta' = \beta_+$ as defined in Eq. (1.54). This finishes the proof.

□

Again, the error $\epsilon$ here is not the error of a particular thermal operation not being able to extract work. It is an error which represents our confidence on a particular thermal operation existing or not. That is, if the energy of the bath is too low (which happens with very small probability), the number of bath states we need to achieve the transition is not available at the energy scales that we have access to. More energy would have to be pumped into the bath to make it possible. The same reasoning applies to the error probability in Theorem 3.

Of the three terms in Eq. (1.67), one is a change of partition function with respect to the infinite-size partition function, the other one is the $\infty$-order Renyi free energy at infinite size (which we will define in Section 1.4.1 below), and the last one is a term that is always positive, and converges to zero in the limit of infinite size. Unlike the previous case, this is not equal to just a Renyi free energy with a shifted temperature.

In Fig. 1.4 we show the maximum extractable work and the minimum work of formation for a particular example, as a function of the modified temperature $\beta'$. We also show an example of the value of both works for a given $\epsilon$ error.

## 1.4 The infinite heat bath limit

We now focus on the particular limit that will be the regime on which we will operate for the rest of the thesis, that in which we can approximate our bath to be of infinite size (or dimensionless volume), and effectively the heat capacity is infinitely large, compared to $C \to \infty$. This limit is equivalent to taking $\gamma \to 0$. When this is done, the thermomajorization diagrams for each energy simplifies dramatically, as the dependence on the total energy disappears.

First, we note what happens to the density of states: it becomes a simple exponential function of the energy of the bath

$$\Omega(E - E_i) \simeq \Omega(E) e^{-\beta E_i}. \tag{1.73}$$

Analogously, the total energy distribution $p(E)\Omega(E)$ defined in Eq. (1.6) in Section 1.1.1 turns into a very peaked Gaussian, tending to a Dirac delta function.

The points that make up the thermomajorization diagram, which were defined in Eq. (1.50) for different $E_{\text{tot}}$ all simplify to the same diagram

$$\Big\{ \Big( \sum_{i=1}^{k} e^{-\beta E_i}, \sum_{i=1}^{k} p_i \Big) \Big\} \ \forall k \in \{1, ..., n\}, \tag{1.74}$$

which is independent of the total energy. This is a diagram made up of a convex curve that starts at $(0, 0)$ and has an endpoint at $(Z_S, 1)$. We show examples of such diagrams, and different transitions that may be possible, in Fig. 1.5.

Therefore, the criteria for when a transformation is possible between quasiclassical states simplifies dramatically if we can implement thermal operations involving an infinite heat bath. On top of that, unlike in the sections above, the answer one gets out of it is always conclusive, without some small probability of error. We summarize this in the following result, which is the central one of [89] and will be the basis of many of the results of the next chapter.

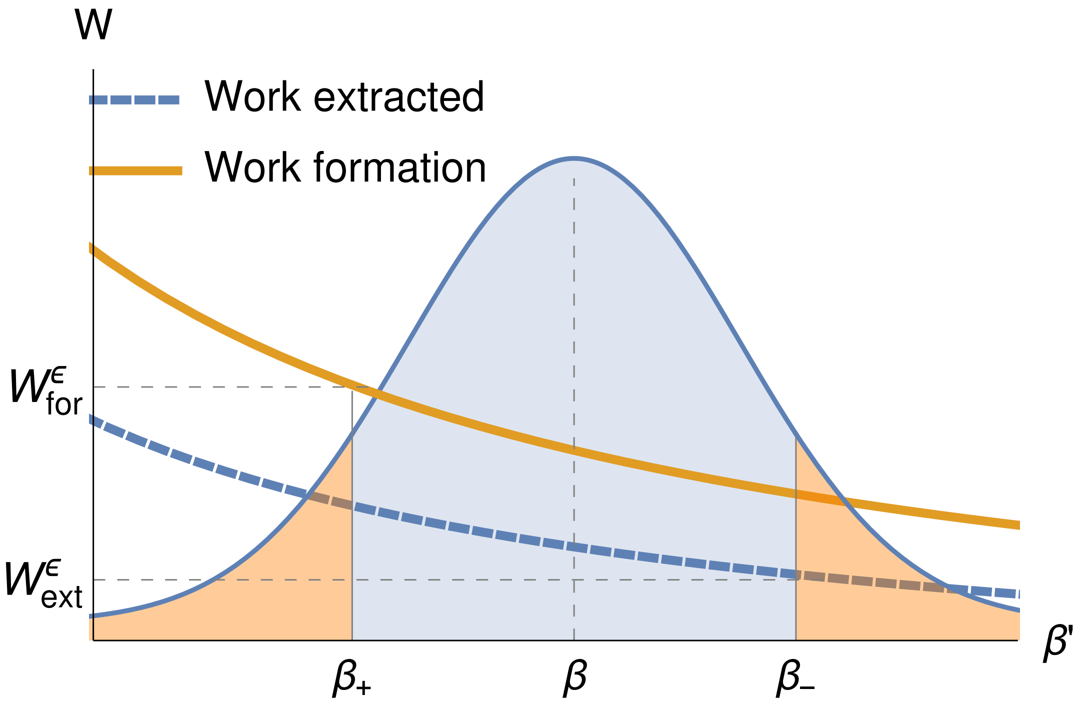

Figure 1.4: We show the curves for the maximum work extracted and minimum work of formation for a state $\rho$, given each particular $\beta'$ . The distribution of total energies (and hence the distribution of $\beta' = \beta - \gamma E$) is the Gaussian curve, for which a cut in the tails gives the values of effective temperatures $\beta_-$ and $\beta_+$ that determine the work of formation and the extractable work given some small error probability, whose value is equal to the area of the orange region. The orange region represents states of the bath for which the energy is either too large or too small that the transformations we want to implement via a thermal operations may not be possible. The width of this Gaussian is inversely proportional to the heat capacity of the bath.

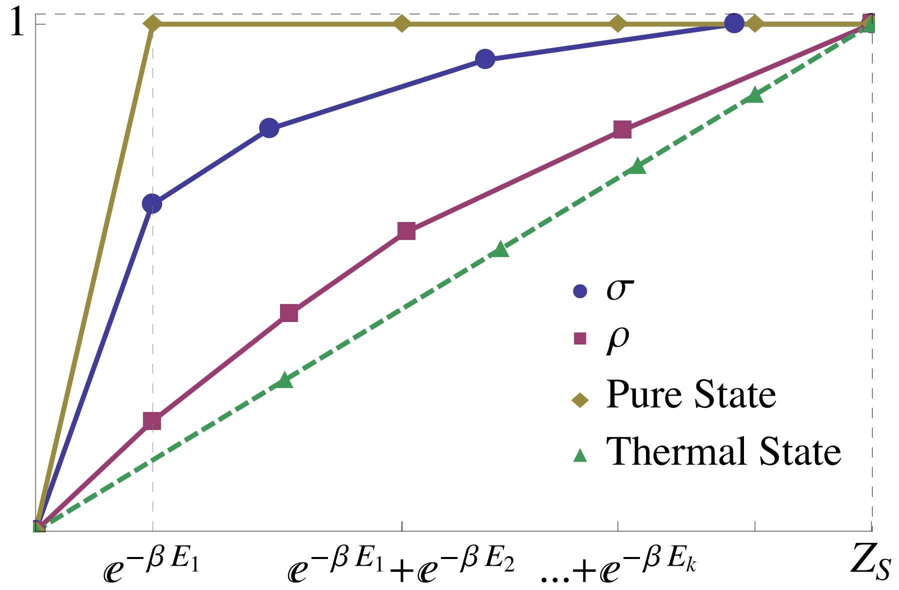

Figure 1.5: We show the $\beta$-ordered thermomajorization diagrams for various states of the system. Note that different states may have different $\beta$-orderings and the markings on the $x$-axis correspond to one particular $\beta$-ordering. The curves always end at $(Z_S, 1)$. The thermomajorization criteria states that we can take a state to another under thermal operations if and only if the curve of the initial state is above that of the final state. Hence, given that $\rho$ and $\sigma$ are quasiclassical states, there is a set of thermal operations such that $\sigma \overset{TO}{\rightarrow} \rho$, but not for the reverse transition $\rho \rightarrow \sigma$.

**Theorem 5.** *The transition between two quasiclassical states $\rho$ and $\sigma$ is possible via thermal operations if and only if the thermomajorization diagram of $\rho$ lies above that of $\sigma$. When that is the case, we say that $\rho$* thermomajorizes *$\sigma$.*

*Proof.* The proof follows from Lemma 3 and the fact that all thermomajorization diagrams collapse to the same one as can be seen from Eq. (1.50). □

The expressions for the extractable work and the work of formation simplify significantly too. Let us note that by taking the limit of infinite heat capacity one obtains $\beta_{\pm} \to \beta$. Therefore

$$\lim_{C\to\infty} W_{\mathrm{e}}(\rho) = F^{\beta}_{\mathrm{min}}(\rho), \tag{1.75}$$

and also

$$\lim_{C\to\infty} W_{\mathrm{f}}(\rho) = F^{\beta}_{\mathrm{max}}(\rho), \tag{1.76}$$

where the min and max free energies are defined as in Eq. (1.62) and (1.68) respectively.

These free energies are related to particular measures of information: the classical Renyi divergences, which are defined as

**Definition 11** (Renyi divergences)**.** *Given two classical probability distributions $p$ and $q$, such that the support of $p$ (that is, the set of terms that are nonzero) is contained within the support of $q$, we define the $\alpha$-Renyi divergence as*

$$D_{\alpha}(p||q) = \frac{1}{\alpha-1}\log\sum_{i=1}^{n}\frac{p_i^{\alpha}}{q_i^{\alpha-1}} \;\; \forall\alpha\in\mathbb{R} \tag{1.77}$$

*If the support of $q$ is larger than that of $p$, $D_{\alpha}(p||q)\to\infty$.*

In particular, if we take $q$ in the definition to be the thermal distribution with temperature $\beta$ (which we define as $q_{\beta}$), we have that

$$\beta F^{\beta}_{\mathrm{min}}(\rho) = D_0(p||q_{\beta}) + \log Z_S \tag{1.78}$$

and

$$\beta F^{\beta}_{\mathrm{max}}(\rho) = D_{\infty}(p||q_{\beta}) + \log Z_S \tag{1.79}$$

so we can see how in this limit, measures of information relevant in the single-shot regime[2] of information-theoretic protocols appear in the context of this resource theory of athermality.

---

[2] This regime is that in which information-theoretic tasks happen only at the level of single copies of the messages, and single uses of the channels.

The usefulness of these measures of information in the context of information theory and cryptography is beyond the scope of this thesis, but we refer the reader to [182] for a more thorough account of classical applications, and to [178] for the quantum versions.

In the following, for quasiclassical states such as $\rho = \sum_{i=1}^{n} p_i |E_i\rangle\langle E_i|$ and $\sigma = \sum_{i=1}^{n} q_i |E_i\rangle\langle E_i|$, we may indistinctively write the Renyi divergence as either $D(p||q)$ or $D(\rho||\sigma)$.

### 1.4.1 Sufficiency of the Renyi divergences

In [28] it was shown that the full set of Renyi divergences ranging in $\alpha \in [0, \infty]$ can be used to give another criterion for knowing when thermodynamical transitions are possible. One may think of allowing an extra ingredient to the resource theory: a catalyst. We define this as a system (which for simplicity we will take to be in a quasiclassical state) such that it aids in a particular transition, but when the thermal operation finishes, it is returned in its original state. In the literature these catalyst-aided processes are given the name *catalytic thermal operations*. That is, we have that the transition

$$\rho \xrightarrow{CTO} \sigma \tag{1.80}$$

is possible if and only if there exists a catalyst system with Hamiltonian $H_C$ in a state $\sigma_C$

$$\rho \otimes \sigma_C \xrightarrow{TO} \sigma \otimes \sigma_C. \tag{1.81}$$

The central result of [29] is the following theorem, which encodes the extra power that having access to arbitrary catalysts yields

**Theorem 6.** *The transition between quasiclassical states $\rho$ and $\sigma$ given by*

$$\rho \xrightarrow{CTO} \sigma \tag{1.82}$$

*is possible under catalytic thermal operations if and only if*

$$F_\alpha^\beta(\rho) \geq F_\alpha^\beta(\sigma) \ \ \forall \alpha \ s.t. \ 0 \leq \alpha \leq \infty, \tag{1.83}$$

*where we define the Renyi free energies as*

$$\beta F_\alpha^\beta(\rho) = D_\alpha(\rho||\tau_\beta) + \log Z_S \tag{1.84}$$

That is, the transition is possible if and only if all the Renyi divergences with respect to the thermal state (which can all be thought of as different measures of athermality) do not increase after the catalytic thermal operation.

This idea of a catalyst gives a natural extension of the resource theory, and may be useful, for instance, in proving fundamental limitations for the efficiency of small-scale heat engines [193] under some conditions, if one considers a catalyst as an engine that must be returned to its original state at the end of a cycle.

### 1.4.2 Work of transition in the infinite bath limit

Another quantity that we are now able to compute easily is the work of transition between two arbitrary quasiclassical states. This is based on the thermomajorization criteria, so that in this case the answers we get for these works are also conclusive, without some small probability of the criteria giving the wrong answer.

As we illustrate in Figure 1.6, the effect of appending a pure state of the battery to $\rho$ is equivalent to stretching the thermo-majorization curve by a factor of $e^{-\beta W}$, and tensoring by the corresponding zero-energy state to $\sigma$ does not change the curve [89]. In both cases the $\beta$-order is preserved, and the new curves will have a lengthened $x$-axis $\left[0, Z_S\left(1+e^{-\beta W}\right)\right]$. These different stretchings can serve to place the curve of $\rho$ just above that of $\sigma$, in which case $W$ will be the work of transition.

In thermal operations, the horizontal distance between a state's thermo-majorization curve and the $y$-axis is again a monotone for each value of $y \in [0,1]$. We denote these by $\tilde{L}_y$ and, as before, they never decrease under thermal operations, which can be seen from the statement of the thermomajorization criterion. In particular, for block-diagonal $\rho$, we have that at the elbows of the diagram:

**Definition 12** (Horizontal monotones)**.**

$$\tilde{L}_{y_k}\left(\rho\right) = \sum_{i=1}^{k} e^{-\beta E_i},\ \textit{for}\ y_k = \sum_{i=1}^{k} p_i, \quad 1 \leq k < \textit{rank}\left(\rho\right), \tag{1.85}$$

$$\tilde{L}_1\left(\rho\right) = \sum_{i=1}^{\textit{rank}(\rho)} e^{-\beta E_i}, \tag{1.86}$$

*where all sums have been properly $\beta$-ordered.*

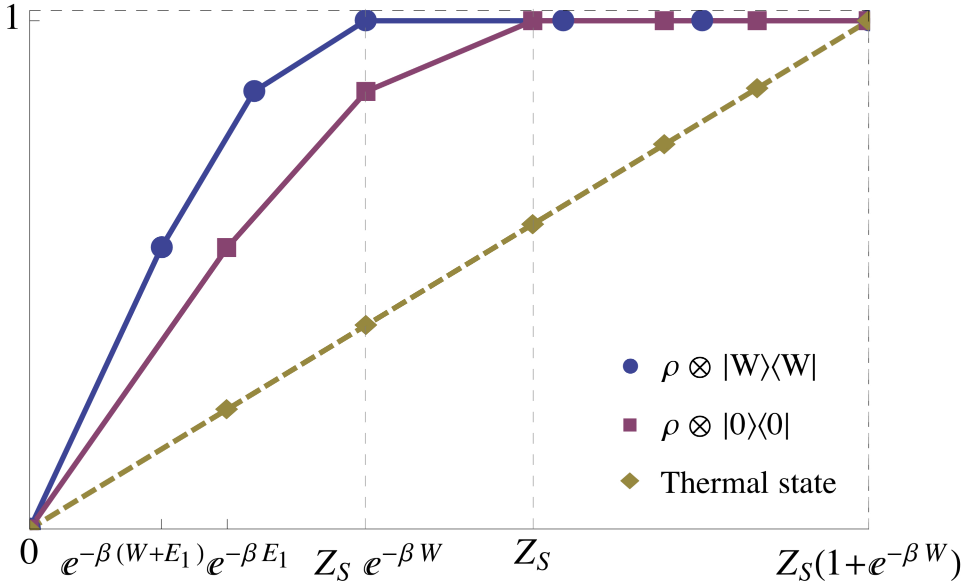

Figure 1.6: We show the thermo-majorization curves of a qutrit system to which a work qubit in one of two pure states has been tensored. Adding this work system takes $Z_S \to Z_S\left(1+e^{-\beta W}\right)$, extending the $x$-axis. When we tensor with the ground state to form $\rho \otimes |0\rangle\langle 0|$, the curve is the same as for $\rho$ alone (the purple curve), but when the excited state is tensored, there is a change in the energy levels of the $\beta$-ordering, and as a result the curve of $\rho$ is compressed by a ratio of $e^{-\beta W}$ (the blue curve). We can see this form the fact that the vertical position of the elbows coincides between the two, but that the horizontal does not. We also show, for completeness, the thermal state of the system-battery together. Note that by construction the blue and purple curves represent states without full support.

We can think of these monotones as not defined only in the particular $y_k$ that represent the elbows of the diagram, but in the whole range $y \in [0,1]$, representing the distance to the vertical axis of every point in the diagram. We hence write instead the set of monotones $\tilde{L}_y$ for any $y \in [0,1]$. A diagramatic illustration on this monotone is shown in Fig. 2.6 in the next chapter.

These allow us to define the work of transition between two classical states.

**Lemma 5.** *Given two quasiclassical states $\rho$ and $\sigma$, under thermal operations:*

$$e^{-\beta W_{\rho\to\sigma}} = \max_{y\in\mathcal{D}(\sigma)} \frac{\tilde{L}_y(\rho)}{\tilde{L}_y(\sigma)}, \tag{1.87}$$

*where $\mathcal{D}(\sigma)$ is the set of vertical coordinates in the diagram of the elbows of the final state $\sigma$.*

*Proof.* To prove this we use geometrical properties of the thermomajorization diagrams. First note that we have that

$$e^{-\beta W_{\rho\to\sigma}} = \max_{y\in\{0,1\}} \frac{\tilde{L}_y(\rho)}{\tilde{L}_y(\sigma)}, \tag{1.88}$$

as the number is defined by how much we have to compress in the horizontal direction the initial state in order for its thermomajorization diagram to be just above that of the final state. This can be seen by the effect that tensoring in a battery system has on the diagram, as shown in Fig. 1.6.

We still have to show that only the subset of points $\mathcal{D}(\sigma)$ may be used in the optimization. Let $s_0 = 0$ and $s_k = \sum_{j=1}^{k} q_j$ for $1 \le k \le \operatorname{rank}(\sigma)$. Then, for $1 \le j \le \operatorname{rank}(\sigma)$, as the thermomajorization diagram of $\sigma$ is a straight line on the interval $[s_{j-1}, s_j]$ and the thermomajorization diagram of $\rho$ is concave:

$$\max_{y\in[s_{j-1},s_j]} \frac{\tilde{L}_y(\rho)}{\tilde{L}_y(\sigma)} \le \max_{r\in[0,1]} \frac{r\tilde{L}_{s_{j-1}}(\rho) + (1-r)\,\tilde{L}_{s_j}(\rho)}{r\tilde{L}_{s_{j-1}}(\sigma) + (1-r)\,\tilde{L}_{s_j}(\sigma)}. \tag{1.89}$$

From the fact that the curves I convex, it can be seen that the maximum value occurs at either $r = 0$ or $r = 1$. We can thus replace the inequality in Eq. (1.89) with an equality. Hence, in the optimization in the lower bound of Eq. (1.89), the result is always one of the extrema of the interval, corresponding to one of the elbows of $\sigma$ in the diagram. Following the same reasoning for every single interval $[s_{j-1}, s_j]$, we see that in Eq. (1.88) it suffices to maximize over $y \in \mathcal{D}(\sigma)$.

□

This result means that calculating the work of transition is a computationally easy task given the thermomajorization diagrams. Previously, in [146] it was shown that this quantity is the solution to a linear program, which can be solved efficiently by standard methods [27].

## 1.5 Changing the Hamiltonian

Throughout this section we have been assuming that the Hamiltonian of the system stays constant. It may be desirable, however, to introduce a controlled way of being able to change it. This way we can account for processes in which the system is driven through a controlled Hamiltonian, which overall may not be completely cyclical. This will become more important in later sections in connection to fluctuation theorems.

How can this be done, while still being consistent with the conservation of energy? The idea is to introduce an additional ancilla system that acts as a control parameter. This can be simplified to a two-level system $X$ with degenerate energy levels which acts as a switch [89].

Now the total Hamiltonian is

$$H = H_S \otimes |0\rangle\langle 0|_X + H'_S \otimes |1\rangle\langle 1|_X + H_B + H_W \ , \tag{1.90}$$

and energy conservation reads $[V, H] = 0$, where $V$ is the global unitary when we include the switch. Note that the Hamiltonian of Eq. (1.90) is not of the same form as that in which we bring in a battery.

We shall impose that the initial state of the switch is $|0\rangle_X$ and the global unitary $V$ performs the switching

$$V\left(\rho_{SBW} \otimes |0\rangle\langle 0|_X\right) V^\dagger = \rho'_{SBW} \otimes |1\rangle\langle 1|_X \ , \tag{1.91}$$

for any $\rho_{SBW}$. A unitary that follows Eq.(1.91) for any input state $\rho_{SBW}$ is

$$V = U \otimes |1\rangle\langle 0|_X + \tilde{U} \otimes |0\rangle\langle 1|_X \ , \tag{1.92}$$

where $U$ and $\tilde{U}$ are unitaries on system, bath and battery. Some simple algebra steps show that the condition $[V, H] = 0$ implies the following relation

$$U(H_S + H_B + H_W) = (H'_S + H_B + H_W)U \ , \tag{1.93}$$

which can be seen as a generalization of the commutation relation in Eq. (1.34). Therefore, the reduced map on system, bath and battery can be written as

$$\Gamma_{SBW}(\rho_{SBW}) = U\rho_{SBW}U^{\dagger}\ , \tag{1.94}$$

where the unitary $U$ does not necessarily commute with $H_S + H_B + H_W$ nor $H'_S + H_B + H_W$ but satisfies Eq. (1.93).

When the Hamiltonian can change along the process, we do not exactly have the constraint which states that the thermal operation preserves the Gibbs state, but instead (1.16) now transforms into

$$T(e^{-\beta H_S}) = e^{-\beta H'_S}, \tag{1.95}$$

which is only equivalent to the Gibbs-preservation condition if the partition functions at the beginning and at the end coincide.

If they do not coincide, some care needs to be taken in interpreting (1.95). It is known that via a quasistatic process one can perform the transition $\tau'_S \to \tau_S$ while extracting an amount of work given by $\log \frac{Z'_S}{Z_S}$, thus extracting work from the thermal state via the thermal operation of Eq. (1.95). If we add a battery state with that much amount of work (which effectively changes the energy levels by a constant amount), it can be seen that the conditions above allow for the thermal state of one Hamiltonian to turn to the thermal state of the other Hamiltonian. Otherwise, the constraint cannot be interpreted as the effect of the thermal operation on a particular map, but just as an abstract linear constraint, which when focusing on quasiclassical states turns into

$$\sum_{i=1}^{n} P(j|i)e^{-\beta E_i} = e^{-\beta E_j}\ \forall\, j, \tag{1.96}$$

which is the equivalent of the Gibbs-preservation condition defined in Theorem 1.

For the rest of the thesis, and in particular in regards to fluctuation relations in Chapter 3, we shall be assuming that the Hamiltonian of the system may not remain constant after a thermal operation. When it is not, it will be because the switch qubit and the construction of Eq. (1.90) will be in use.

## 1.6 What about quantum coherence?

Within this chapter, and throughout most of this thesis, we focus on a subset of states, which are the quasiclassical states. An obvious question is: what happens when states have coherence in the energy eigenbasis between non-degenerate energy levels? It turns out that dealing with the general behaviour of transitions between such states is a much more difficult problem, for which a general answer is not yet known. Partial results have been obtained, however, by thinking of this coherence in energy in terms of another resource-theoretic framework: that of *asymmetry* [120, 121]. Indeed, a productive perspective is to think of states with coherence in energy as states that break a symmetry associated to the action of the time translation operation from Eq. (1.18). That is: states with coherence are not invariant under the action of time-translations.

In particular, with this perspective one can derive additional necessary constraints that the pairs of states with coherence must obey in order for the transition to be possible. These can be found in the works [115, 116, 49], and can be paired in two sets:

- By computing a distance from a state to its decohered quasiclassical version. The simplest example the relative entropy of an arbitrary (not quasiclassical) state $\rho$ to its quasiclassical version $\Delta_S(\rho)$

  $$D(\rho||\Delta_S(\rho)) = \mathrm{Tr}[\rho(\log(\Delta_S(\rho)) - \log(\rho)], \tag{1.97}$$

  which can only decrease as due to the contractivity property of the relative entropy under quantum maps, given a thermal operation $T(\cdot)$ we have

  $$D(\rho||\Delta_S(\rho)) \geq D(T(\rho)||T(\Delta_S(\rho))) = D(\sigma||\Delta_S(\sigma)). \tag{1.98}$$

  Similar monotones can also be defined via other Renyi divergences [115].

- By exploiting the two key properties of time-translation symmetry and preservation of the Gibbs state [116]. The proof is beyond the scope of this section, but we show the result for completeness. Let us write $\rho = \sum_{i,j} \rho_{ij} |E_i\rangle\langle E_j|$ so that $\rho_{ij}$ represent the coherent terms when $E_i \neq E_j$. The following bound holds when $\rho \overset{TO}{\to} \sigma$:

  $$|\sigma_{kl}| \leq \sum_{i,j,E_i<E_k} |\rho_{ij}| e^{-\beta E_k - E_i} + \sum_{i,j,E_i>E_k} |\rho_{ij}|, \tag{1.99}$$

where the sum is over pairs of $i, j$ such that $E_i - E_j = E_k - E_l$.

Even if the problem of coherence is an important one thermodynamically, it may not be so much if our focus is that of work extraction. It is known that no work can be extracted from coherence in the absence of another source of coherence to help us, a *reference frame* [115], and even in such a case the optimal way of extracting work from coherence in general is far from clear [104].

## 1.7 Limitations of thermal operations

Above we have described most of the building blocks of the resource theory of athermality. Important questions remain: what kind of processes fit into the set of free operations? And exactly what physics is this framework useful for? To try to answer these we now examine in more detail some of the limitations of the assumptions made through this chapter.

### Energy conservation

From a resource-theoretic perspective, the condition of energy conservation exists in order to be able to keep track of the energy flows. This usually applies in the macroscopic regime because all the systems are coupled through their boundaries, which involve scales of energy much lower than those in the bulk, effectively coupling all the components very weakly to each other.

This condition also applies to the case in which the quantum systems are weakly coupled to the heat bath (this is how more explicitly in Lemma 9 in Chapter 4). The thermodynamics of these physical situations is very well understood [53, 165, 12, 34], and the master equation formalism can be used to describe their behaviour in detail.

In the quantum regime, however, weak coupling is not always a good approximation. In fact, there are models in which such energy conservation holds, but which are not weakly coupled. A prominent example is the resonant Jaynes-Cummings model after making the rotating wave approximation [96]. In it we have a bosonic bath and a two level system (which we take to have energies $E_l$ and $E_k$ s.t. $E_k - E_l = \hbar\omega$), and the coupling Hamiltonian is given by

$$H_I = \Omega(a \otimes |E_k\rangle\langle E_l| + a^\dagger \otimes |E_l\rangle\langle E_k|), \tag{1.100}$$

where $\Omega$ is the coupling constant, $a$, $a^\dagger$ are the bosonic creation and annihilation operators of a mode with frequency $\omega$. We can see that the effect of this interaction is that of taking a photon and exciting the two level atom, or the opposite of de-exciting the atom and emitting a photon, and hence it involves processes in which energy is transferred from one system to another exactly. That is, we have that

$$[H_I, H_S + H_B] = 0, \tag{1.101}$$

where $H_S = \sum_i E_i|E_i\rangle\langle E_i|$ and $H_B = \omega a^\dagger a$. The set of thermal operations hence includes the action of all interaction Hamiltonians that obey this commutation property. For a thorough analysis of the thermodynamic power of interactions on two energy levels such as this Jaynes-Cummings interation, we refer the reader to [114].

We can also think of other interactions between system and bath in which they interact strongly only during part of the process. For instance, we could have a system far apart from a bath, bring it closer and make it interact strongly, and then take it away again. This is a kind of process that may be included within thermal operations if we take into account that there may be some additional control unit needed to power this time-dependent interaction, which may consume some sort of thermodynamical resource. The resource-theoretic account of the amount of control that such a process requires is a technically challenging question and is a subject of current study. Recent progress on this can be found in, for instance, [29, 194].

On top of all this, we can also think of processes, such as those that involve strong coupling at all times [103, 167, 138]. These may indeed not be straightforwardly included within the framework of thermal operations as free operations. However, relevant questions to consider are: in so far as these processes deviate from the set of free operations, what is the resource-theoretic value of such processes? Or how do we quantify the degree of strong coupling in terms of measures of athermality? These questions are up to date unexplored, and are one of the potential avenues of expansion of the resource theoretic approach.

### General unitaries

Another objection to the constraints of thermal operations goes in the opposite direction: that in a way we are allowing for too much control. The assumption is that one can access any particular unitary, with the only condition having to be energy conservation. This will mean that we include unitaries that are far from being physically realizable, and that may for instance allow for a really fine-grained control of the microstates of the bath.

While this is indeed the case, the limitations for thermodynamical processes that the resource theory constraint imposes will then be universal, for any kind of process that obeys the assumptions. In that sense one can think of this framework as a fundamental one, in a way similar to which coding theorems in information theory give fundamental bounds to the cost of communicating and compressing information.

In connection to this point, the following question has been asked recently: if we restrict the set of operations in some physically motivated way, such that not all unitaries are allowed, how much control do we actually lose over which transitions are possible? A complementary question is: how much fine-grained control is needed in order to recover thermomajorization as a criteria for when a transition between states is possible?

There is an increasing body of work aiming at addressing these issues, including [141, 114, 191, 125]. The restrictions that have been considered to be physically relevant are, for instance, limiting to two-level thermalization processes and adiabatic level transformations, to general operations on two levels only, or to operations with some locality restriction. For instance, in [141] a set of operations smaller than thermal operations in which thermomajorization is recovered is given. On the other hand, [114] explores cases in which the full thermomajorization is not recovered, and a different criteria must be given.

### System and bath are initially in a product state

A final objection one can raise about the assumptions of thermal operations is that fixing the system to be uncorrelated with the bath before the process starts can be limiting. It is known that in many cases system-bath correlations are important, in particular when one deals with strong coupling and non-markovianity, which have non-trivial thermodynamic effects [39, 143].

This product assumption is usually taken in the context of weak coupling and the Born-Markov approximations, although rather than the exact behaviour in the limit, it has to be thought of more as a useful idealization [152].

When correlations are present, the thermodynamic behaviour displayed may change drastically. Indeed, correlations between system and bath are known to allow for processes such as anomalous heat flows [16, 57], and in general mean that the second law does not hold, and that corrections to it must be included [187, 25].

These generic facts indicate that these correlations must be understood as an extra resource that is brought in from the start, different in nature to for instance bringing in an external source of work. Given this, one may not look at this assumption as an objection, but as a possibility: a natural question to ask, which remains mostly unanswered up to date, is how to account properly for the resource that these initial correlations represent. A potential approach to this question is to find out in which way exactly can these correlations be useful in extracting work, a subject that has been explored recently in various settings [71, 140].

## 1.8 Summary

In this chapter we have introduced the resource theory, by outlining the ingredients and showing mathematical statements that explain the structure and power of the framework. The perspective taken has been that of introducing first the heat bath as a finite physical object, and explore the limitations associated to its size. We define the notion of deterministic work and explain what does it mean to extract it, and gave expressions that limit the amount that can be extracted, provided we accept the answer may be wrong with small probability.

We then took the common assumption of an infinite heat bath and showed how from it one can recover the standard results of thermomajorization and work extraction from [89]. We also explored particular cases such as degenerate energy spectrum and catalysts, went over the difficulties associated with quantum coherence and critically examined the limitations of the framework.

# Chapter 2

# Fluctuations of states

We now follow the results of [6] and introduce another kind of transition between states in the resource theory, beyond the one contained in Theorem 5 regarding thermomajorization.

If the quasiclassical state $\sigma$, is not thermo-majorized by $\rho$, and hence there exists no free thermodynamical process (that is, thermal operation) that converts $\rho$ into $\sigma$, we know the transformation is still possible provided sufficient work is supplied. We have seen in the previous chapter that one can compute the work required (or gained) from this transition using thermo-majorization diagrams [89], and also via a linear program [146]. Suppose however, we want to make a transition from $\rho$ to $\sigma$, and it requires work which we cannot, or do not wish to, expend. Can we still nonetheless make the transition without work with some probability $p$ rather than with certainty? And if so, what is the highest probability, $p^*$, that can be achieved? In particular, given $\rho$ and $\sigma$, we are interested in maximizing $p$ in the following process:

$$\rho \longrightarrow \rho' = p\sigma + (1-p)\, X, \tag{2.1}$$

with $X$ being some arbitrary state.

This can be thought of as a fluctuation of a system's state, as the transformation is only probabilistic. Within the study of thermodynamics for small systems, a common focus is in regards to the probabilistic fluctuations of the work as a random variable [94, 46, 173, 171]. Fluctuation relations such as the Jarzynski equality [94] and Crooks' theorem [46], developed under the paradigm of stochastic thermodynamics, have been used to calculate and give the key features of the work fluctuations of non-equilibrium processes. These will be the subject of

Chapter 3, but the idea behind the results of the present chapter is that investigating fluctuation in a system's state provides a natural, complementary question. As we will see, some of the fundamental limitations in the context of fluctuations of states resemble work fluctuation relations.

Here, we will upper bound the maximum probability of a fluctuation between any given $\rho$ and $\sigma$. When $\sigma$ is quasiclasssical, we will show that this bound can be achieved and furthermore, that there exists a two outcome measurement that can be performed on $\rho'$ such that we obtain $\sigma$ with the maximum probability $p^*$. Measurements for which the outcome is accessible have however a thermodynamic cost, related to the work we need to erase the record of the measurement outcome [21]. We will show that such a measurement can be performed, although for now we take Eq. (2.1) as our primary goal, defining what we mean by a fluctuation of a state. We will discuss measurements more in detail in Section 2.2.3.

Some of the central results of this section are similar in form to [185] which considers the analogous problem of probabilistic pure state entanglement manipulation using Local Operations and Classical Communication (LOCC). However, some important differences are found: first of all, the transformations under LOCC go in a different direction, as there one can bring in separable states for free, and the expensive states are the most locally mixed ones (that is, those with more entanglement). As a consequence, most of the proof techniques had to be adapted. Another important difference is that in the resource theory of entanglement measurements do come for free, so the considerations regarding the erasure cost do not apply there. It should also be noted that in entanglement manipulation, the maximum probability achievable will in some cases be zero, something that as we will see does not happen under thermal operations.

## 2.1 Probability of transition under noisy operations

Before investigating probabilistic transitions of states in the context of thermal operations, we shall first focus on a simpler, special case, that of noisy operations. This is a particular instance of a thermodynamic resource theory in which the Hamiltonian of the system under consideration is trivial and energy does not play a role, only purity does. A reason to introduce this framework at this point is that the proof of the statements for this simplified case will be used in the proofs for the more general case of non-trivial Hamiltonians which will follow.

Noisy operations were first defined in [88] where the problem of whether a transition between two given states under a particular set of operations was considered. In this resource theory, the following general operations are allowed by definition: *i)* a system of any dimension in the maximally mixed state can be added, *ii)* any subsystem can be discarded through tracing out and *iii)* any unitary can be applied to the global system. We shall use $\eta_i$ to denote the eigenvalues of $\rho$ and $\zeta_i$ to denote those of $\sigma$. For a definitive review of noisy operations, see [80]. The motivation for them is to have a general resource-theoretic model of processes in which noise, in the form of maximally mixed states, are for free, but where energy or quantum coherence are not necessarily a concern.

Given any two states, $\rho$ and $\sigma$, it was shown in [88] that the transition from $\rho$ to $\sigma$ is possible under noisy operations if and only if the spectrum of $\rho$ majorizes the spectrum of $\sigma$ (written $\rho \succ \sigma$). Recall that we first defined majorization in Def. 10. That is, if we list the eigenvalues of $\rho$ and $\sigma$ in decreasing order and denote these ordered lists by $\vec{\eta} = \{\eta_1, \ldots, \eta_n\}$ and $\vec{\zeta} = \{\zeta_1, \ldots, \zeta_n\}$ respectively, the transition is possible if and only if:

$$V_l(\rho) \geq V_l(\sigma), \quad \forall l \in \{1, \ldots, n\}, \tag{2.2}$$

where:

$$V_l\left(\rho\right) = \sum_{i=1}^{l} \eta_i. \tag{2.3}$$

An important point to note is that here we can focus on all quantum states, no matter in which basis they are diagonal. The fact that no energy is involved, and that arbitrary unitaries are free operations, means that we do not need to focus on a particular basis, or a particular notion of quasiclassical states. Rather than that, we find that only the spectrum of the states matters in this context.

The analogue of thermomajorization diagrams are the Lorenz curves, which are a useful tool for visualizing the states (see Fig. 2.1 for an example). The first mention of this was given in Section 1.2.2, where we saw that thermomajorization collapses to majorization when the Hamiltonian of the system of interest is fully degenerate. Indeed, degenerate energy thermodynamics can be thought of as part of this resource theory of noisy operations.

For a given state $\rho$, its Lorenz curve is formed by plotting the points:

$$\left\{\left(\frac{k}{n}, \sum_{i=1}^{k} \eta_i\right)\right\}_{k=1}^{n}, \tag{2.4}$$

and connecting them piecewise linearly (together with the point $(0,0)$) to form a concave curve. If $\rho$ majorizes $\sigma$, the Lorenz curve for $\rho$ is never below that of $\sigma$.

The functions defined in Eq.(2.3) are monotones of the theory, only decreasing under noisy operations. The theory of majorization is very well developed within the mathematical literature, and for good general references we refer the reader to [119, 80].

### 2.1.1 Non-deterministic transitions

We now move to the main focus of this section, which are transitions in which the majorization conditions are not necessarily fulfilled. Here, rather than transforming $\rho$ to $\sigma$ with certainty, it will only happen with some probability as defined in Eq. (2.1). In particular, we want to find an expression for the maximum probability, $p^*$, that can be achieved. Adapting the techniques from [185] the following theorem can be shown:

**Theorem 7.** *Suppose we wish to transform the state $\rho$ to the state $\sigma$ under noisy operations. The maximum value of $p$ that can be achieved in the transition:*

$$\rho \xrightarrow{NO} \rho' = p\sigma + (1-p)\, X, \tag{2.5}$$

*is given by:*

$$p^* = \min_{l\in\{1,\ldots,n\}} \frac{V_l\,(\rho)}{V_l\,(\sigma)}. \tag{2.6}$$

*Proof.* The proof is split into two parts: first we apply Weyl's inequality and the definition of majorization to derive a contradiction if it were possible to achieve a value of $p$ large than $p^*$. Next, we adapt the techniques of [185] to provide a protocol achieving $p = p^*$.

To achieve our first goal we begin by showing that given Eq. (2.5):

$$V_l\,(\rho) \geq p V_l\,(\sigma)\,, \quad \forall l. \tag{2.7}$$

To prove this, we make use of a useful identity for Hermitian matrices called Weyl's inequality. A proof of it can be found in [189, 87]. Given any $n \times n$ Hermitian matrices, $A$, $B$ and $C$

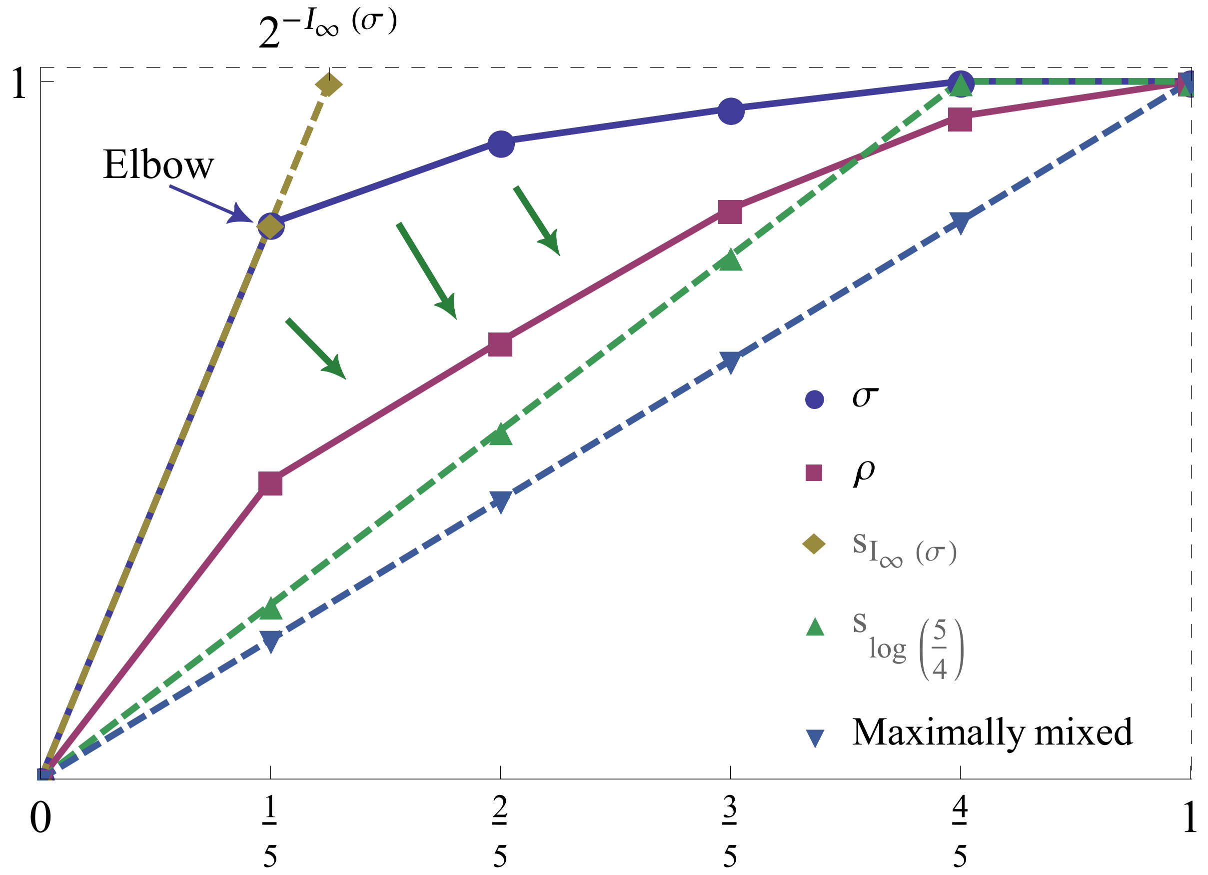

Figure 2.1: *a)* The Lorenz curve for $\rho$ is defined by plotting the points: $\left\{\left(\frac{k}{n},\sum_{i=1}^{k}\eta_i\right)\right\}_{k=1}^{n}$. *b)* The transition from $\sigma$ to $\rho$ is possible under NO as the curve for $\sigma$ is never below that of $\rho$. *c)* The Lorenz curve for a maximally mixed state is given by the dashed line from $(0,0)$ to $(1,1)$. All other states majorize it. *d)* $s_{\log\frac{5}{4}}$ is an example of a sharp state. *e)* $s_{I_\infty(\sigma)}$ is the least sharp state that majorizes $\sigma$, where we define $I_\infty(\sigma) = \log\frac{n}{\xi_1}$, with $\xi_1$ the largest eigenvalue of $\sigma$.

such that $A = B + C$, let $\{a_i\}_{i=1}^n$, $\{b_i\}_{i=1}^n$ and $\{c_i\}_{i=1}^n$ be their respective eigenvalues arranged in descending order. Weyl's inequality then states that:

$$b_i + c_n \leq a_i \leq b_i + c_1 \ \ \forall i. \tag{2.8}$$

Applying this to $\rho'$, $\sigma$ and $X$, we obtain

$$\eta_i' \geq p\zeta_i + (1-p)\, x_n, \quad \forall i, \tag{2.9}$$

where $x_n$ is the smallest eigenvalue of $X$. As $X$ is by definition a positive semidefinite matrix, $x_n \geq 0$ and

$$\eta_i' \geq p\zeta_i, \quad \forall i. \tag{2.10}$$

Hence

$$V_l(\rho) \geq V_l(\rho') = \sum_{i=1}^{l} \eta_i' \geq p \sum_{i=1}^{l} \zeta_i = pV_l(\sigma), \tag{2.11}$$

where the first inequality uses the majorization conditions and the second follows from Eq. (2.10).

Suppose it was possible to achieve a value of $p$ greater than $p^*$ in Eq. (2.6). Then there would exist an $l$ such that $V_l(\rho) < pV_l(\sigma)$, contradicting Eq. (2.7).

To proceed with the protocol that shows that $p^*$ is obtainable, we shall define a few quantities. First, define $l_1$ as the largest $l$ at which the optimization of Eq. (2.6) finds the minimum. That is

$$l_1 = \max\left\{ l : \frac{V_l(\rho)}{V_l(\sigma)} = p^* \equiv r^{(1)} \right\}. \tag{2.12}$$

Then we proceed iteratively and, provided $l_{i-1} < n$, define a series of ratios $r^{(i)}$ as

$$r^{(i)} = \min_{l > l_{i-1}} \frac{V_l(\rho) - V_{l_{i-1}}(\rho)}{V_l(\sigma) - V_{l_{i-1}}(\sigma)}, \tag{2.13}$$

so we have by construction

$$r^{(i)} \sum_{j=l_{i-1}+1}^{l} \zeta_j \leq \sum_{j=l_{i-1}+1}^{l} \eta_j, \quad \forall l > l_{i-1}. \tag{2.14}$$

Now we define a sequence of $l_i$ through these ratios, as

$$l_i = \max\left\{ l : l > l_{i-1}, \frac{V_l(\rho) - V_{l_{i-1}}(\rho)}{V_l(\sigma) - V_{l_{i-1}}(\sigma)} = r^{(i)} \right\}. \tag{2.15}$$

Note that we have $r^{(i)} > r^{(i-1)}$. To see this, first observe that for $a, b, c, d > 0$:

$$\frac{a}{b} < \frac{a+c}{b+d} \Leftrightarrow \frac{a}{b} < \frac{c}{d}. \tag{2.16}$$

Setting:

$$\begin{aligned} a &= V_{l_{i-1}}(\rho) - V_{l_{i-2}}(\rho), \\ b &= V_{l_{i-1}}(\sigma) - V_{l_{i-2}}(\sigma), \\ c &= V_{l_i}(\rho) - V_{l_{i-1}}(\rho), \\ d &= V_{l_i}(\sigma) - V_{l_{i-1}}(\sigma), \end{aligned}$$

so $\frac{a}{b} = r^{(i-1)}$ and $\frac{c}{d} = r^{(i)}$, then:

$$\frac{a+c}{b+d} = \frac{V_{l_i}(\rho) - V_{l_{i-2}}(\rho)}{V_{l_i}(\sigma) - V_{l_{i-2}}(\sigma)} > r^{(i-1)} = \frac{a}{b},$$

where the inequality follows from the definition of $r^{(i-1)}$. Using Eq. (2.16), the claim that $r^{(i)} > r^{(i-1)}$ now follows. Overall, this protocol generates a set of $l_i$ such that $0 = l_0 < l_1 < \ldots < l_k = n$ and a set of $r_i$ such that $p^* = r^{(1)} < \ldots < r^{(k)}$.

Now we split $\rho$ and $\sigma$ into blocks $\rho_i$ and $\sigma_i$ defined as

$$\rho_i = \operatorname{diag}\left(\eta_{l_{i-1}+1}, \ldots, \eta_{l_i}\right), \tag{2.17}$$

$$\sigma_i = \operatorname{diag}\left(\zeta_{l_{i-1}+1}, \ldots, \zeta_{l_i}\right). \tag{2.18}$$

Then from Eq. (2.14) (and the fact that equality occurs when $l = l_i$), each of the $\rho_i$ majorizes each of the $r^{(i)}\sigma_i$. Majorization makes sense because of the $r^{(i)}$ factor in front of $\sigma_i$, which means that the eigenvalues of both blocks add up to the same number. Given this we can perform a sequence of noisy operations in each block such that

$$\rho_i \xrightarrow{NO} r^{(i)}\sigma_i = p^*\sigma_i + \left(r^{(i)} - p^*\right)\sigma_i, \quad \forall i. \tag{2.19}$$

Putting all the blocks together, we see we have arrived at an equation of the form of our goal Eq. (2.5) with $p = p^*$ and defining the blocks of $X$ by

$$X_i = \frac{r^{(i)} - p^*}{1 - p^*}\sigma_i. \tag{2.20}$$

□

Note that as the endpoints of the Lorenz curves coincide at $(1,1)$ and $\eta_1 > 0$, we are guaranteed that $0 < p^* \leq 1$. In particular, we note that when $\rho$ majorizes $\sigma$ the optimization for finding $p^*$ will always find the minimum at the endpoint, where $p^* = 1$, which we expect as the transformation is deterministic.

One may argue against the meaning of Eq. (2.5) as a probabilistic transition, as we do not know whether we have state $\sigma$ or $X$. In order to address this we find a particular binary quantum measurement for which a positive outcome means we obtain the state $\sigma$ with probability $p^*$.

This is a two outcome measurement, with measurement operators $\{\sqrt{M}, \sqrt{\mathbb{I} - M}\}$, where the blocks of $M$ are given by:

$$M_i = \operatorname{diag}\left(\frac{p^*}{r^{(i)}}, \dots, \frac{p^*}{r^{(i)}}\right). \tag{2.21}$$

We need two facts to show that $M$ gives a valid measurement: that it is positive and that the square of the two operators adds up to the identity. We note that in general $0 < \frac{p^*}{r^{(i)}} \leq 1$, making it positive. Hence both $\{\sqrt{M}, \sqrt{\mathbb{I} - M}\}$ are well defined. Regarding the second condition, their squares add up to the identity by definition.

After applying this measurement to $\rho'$ and reading the result, we will have either:

$$\sqrt{M}\,\rho'\sqrt{M}^\dagger = p^*\sigma, \tag{2.22}$$

or

$$\sqrt{(\mathbb{I} - M)}\,\rho'\sqrt{(\mathbb{I} - M)}^\dagger = (1 - p^*)\,X. \tag{2.23}$$

We note a conceptual difficulty: performing this measurement in a way in which we find the outcome is outside of the class of noisy operations and hence costs work. This can be seen from the fact that if a general two outcome measurement is allowed without taking its cost into account, it can be possible to transform $\rho$ into $\sigma$ with probability greater than $p^*$.

As a simple example, if $\rho$ and $\sigma$ are qubits, we can convert $\rho$ into $\sigma$ with certainty using this extra resource. First we take a qubit in the maximally mixed state and measure it in the computational basis. This results in a pure state, either $|0\rangle$ or $|1\rangle$. As these majorize all other qubit states we can use it to obtain any $\sigma$ with certainty. A similar argument can be used for systems of any dimension.

### 2.1.2 Nonuniformity of transition under noisy operations

If it is not possible to deterministically convert $\rho$ into $\sigma$ using noisy operations, to perform the transformation with certainty will cost some resource, in the form of *nonuniformity*, which will be the analogue of work in this context. For instance, if we add some pure states placed in a sufficiently large Hilbert space, we will be able to use this purity to implement transitions that were previously impossible. Adding these additional pure states can be thought of as the analogue of adding work. In addition, if $\rho$ can be converted to $\sigma$ using noisy operations, it may be possible to extract some nonuniformity in the process (e.g. when transforming some maximally mixed states into pure states).

We shall extract or expend the equivalent of work using *sharp states*. These sharp states, as discussed in the next subsection, serve as natural storage units for the nonuniformity resource. We will compute the nonuniformity of transition in terms of a finite set of ratios of monotones. This was already done in [80], but here we also show that the minimization can be done over fewer points.

#### Sharp States

We shall denote the noisy operations equivalent of work described in Def. 6 , the nonuniformity of transition, by $I_{\rho\to\sigma}$ . If nonuniformity must be added, the quantity is negative, while if we can extract nonuniformity, it will be positive. For $|I_{\rho\to\sigma}| = \log\frac{d}{j}$, we define an associated *sharp state* [80] by:

$$s_{|I_{\rho\to\sigma}|} = \mathrm{diag}\Bigg(\underbrace{\frac{1}{j},\dots,\frac{1}{j}}_{j},\underbrace{0,\dots,0}_{d-j}\Bigg). \tag{2.24}$$

That is, a sharp state is a state on a $d$ dimensional Hilbert space that has support only in a $j$-dimensional subspace, in which it is maximally mixed. Appending a sharp state $I_{\log\frac{d}{j}}$ to the system is equivalent to introducing $\log\frac{d}{j}$ units of nonuniformity. See Figure 2.1 for an example of a sharp state's Lorenz curve. The state $s_{|I_{\rho\to\sigma}|}$ is such that:

$$\begin{aligned} \rho\otimes s_{|I_{\rho\to\sigma}|} &\overset{NO}{\longrightarrow} \sigma, && \text{if } I_{\rho\to\sigma}\le 0,\\ \rho &\overset{NO}{\longrightarrow} \sigma\otimes s_{|I_{\rho\to\sigma}|}, && \text{if } I_{\rho\to\sigma}> 0. \end{aligned} \tag{2.25}$$

In terms of Lorenz curves, tensoring a state $\rho$ with a sharp state $s_I$ has the effect of compressing the Lorenz curve of $\rho$ by a factor of $2^{-I}$ with respect to the $x$-axis [89], analogous to what happens with deterministic work in thermal operations.

### Monotones for noisy operations and the nonuniformity of transition

The function $V_l(\rho)$ is equal to the height of the Lorenz curve of $\rho$ at $x = \frac{l}{n}$. An alternative set of monotones, $L_y(\rho)$ where $0 \leq y \leq 1$, can be defined as the shortest horizontal distance between the Lorenz curve of $\rho$ and the $y$-axis at $y$. Note that these functions *never decrease* under noisy operations. In particular

$$\begin{aligned} L_{y_k}(\rho) &= \frac{k}{n}, \text{ for } y_k = \sum_{i=1}^{k} \eta_i, \quad 1 \leq k < \operatorname{rank}(\rho), \\ L_1(\rho) &= \frac{\operatorname{rank}(\rho)}{n}. \end{aligned} \tag{2.26}$$

We will define the set of elbows of the final state $\sigma$ in the same way as in Lemma 5, as $\mathcal{D}(\sigma)$ by

$$\mathcal{D}(\sigma) = \left\{ \sum_{i=1}^{k} \zeta_i \right\}_{k=1}^{\operatorname{rank}(\sigma)}, \tag{2.27}$$

then a transition from $\rho$ to $\sigma$ is achievable with certainty under noisy operations if and only if

$$L_y(\rho) \leq L_y(\sigma), \quad \forall y \in \mathcal{D}(\sigma). \tag{2.28}$$

That it is sufficient to consider only $y \in \mathcal{D}(\sigma)$ will be justified below as a simple consequence of Lemma 6.

In the same way as in the context of thermomajorization and thermal operations, the horizontal monotones, $L_y$, also allow us to quantify the optimal work of transition that is required or extracted in going from $\rho$ to $\sigma$:

**Lemma 6.** *Given two states $\rho$ and $\sigma$, under Noisy Operations:*

$$2^{-I_{\rho\to\sigma}} = \max_{y \in \mathcal{D}(\sigma)} \frac{L_y(\rho)}{L_y(\sigma)}. \tag{2.29}$$

*Proof.* The proof is exactly the same as that of the more general case of thermomajorization and thermal operations, which was given in Lemma 1.87. In particular, it follows if we consider how majorization emerges as a particular case of thermomajorization for degenerate energy levels, as was shown in Section 1.2.2.

□

As $\rho \xrightarrow{NO} \sigma$ is possible if and only if $I_{\rho\to\sigma} \geq 0$, the finite set in Eq. (2.28) is justified.

In the previous work [80] it was shown that it is possible to calculate $I_{\rho\to\sigma}$ by performing an optimization over the ratios calculated at the 'elbows' (see Figure 2.1 for a definition) of both $\rho$ and $\sigma$. What we show in Lemma 6 is that it suffices to consider just the 'elbows' of $\sigma$.

### Bounds on the transition probability

Now we proceed with the result that illustrates the relation between the two concepts we have defined above: work of transition between two states, and the optimal probability of transition.

This relation is illustrated by the following theorem. The quantities $I_{\rho\to\sigma}$ and $I_{\sigma\to\rho}$ can be used to bound $p^*$ as follows:

**Theorem 8.** *Given two states $\rho$ and $\sigma$, under noisy operations:*

$$2^{I_{\rho\to\sigma}} \leq p^* \leq 2^{-I_{\sigma\to\rho}}, \tag{2.30}$$

*where as $p^* \leq 1$, we assume $I_{\rho\to\sigma} \leq 0$. If $I_{\rho\to\sigma} \geq 0$, $p^* = 1$ and the transformation from $\rho$ to $\sigma$ can be done deterministically, potentially extracting a finite amount of nonuniformity.*

*Proof.* We first prove the lower bound by giving a particular protocol which achieves a probability of transition $p = 2^{W_{\rho\to\sigma}}$, which by definition will be smaller than the optimal one. Then, the upper bound is derived by considering properties of the purity of the least resurceful sharp state that majorizes $\rho$.

Assuming $|W_{\rho\to\sigma}| = \log\frac{d}{j}$ for simplicity, and defining $\mathbb{I}_d$ to be the maximally mixed state of a $d$ level system:

$$\begin{aligned}
\rho &\xrightarrow{NO} \rho \otimes \mathbb{I}_d, \qquad (2.31)\\
&= \frac{j}{d}\rho \otimes s_{\log\frac{d}{j}} + \frac{d-j}{d}\rho \otimes s_{\log\frac{d}{d-j}},\\
&\xrightarrow{NO} \frac{j}{d}\sigma \otimes \mathbb{I}_d + \frac{d-j}{d}Y,\\
&\xrightarrow{NO} \frac{j}{d}\sigma + \frac{d-j}{d}\mathrm{Tr}_B Y,
\end{aligned}$$

where $Y$ is the state obtained by applying the second noisy operation to $\rho \otimes s_{\log \frac{d}{d-j}}$. Using this protocol, we obtain something of the form Eq. (2.5) with $p = 2^{I_{\rho\to\sigma}}$ and $X = \mathrm{Tr}_B Y$. As $p^*$ is the maximum value of $p$ obtainable in Eq. (2.5), we derive the lower bound.

We now consider the upper bound and to obtain a useful bound, assume $I_{\sigma\to\rho} > 0$. We define $I_\infty(\rho)$ as the nonuniformity of formation of $\rho$ under noisy operations [50], given by $I_\infty(\rho) = -\log \eta_1 n$, and hence let $s_{I_\infty(\rho)}$ be the least sharp state that majorizes $\rho$ (see Figure 2.1). Note that $I_\infty$ decreases under noisy operations and is additive across tensor products [80]. In terms of the eigenvalues of $\rho$ and $\sigma$:

$$\begin{aligned} s_{I_\infty(\rho)} &= s_{\log(\eta_1 n)}, \\ s_{I_\infty(\sigma)} &= s_{\log(\zeta_1 n)}. \end{aligned} \tag{2.32}$$

By definition, as $I_{\sigma\to\rho} > 0$:

$$\sigma \xrightarrow{\text{NO}} \rho \otimes s_{I_{\sigma\to\rho}}. \tag{2.33}$$

Now, using first the monotonicity of $I_\infty$ and then the additivity:

$$\begin{aligned} I_\infty(\sigma) &\geq I_\infty\left(\rho \otimes s_{I_{\sigma\to\rho}}\right), \quad \text{(monotonicity)} \\ &= I_\infty(\rho) + I_{\sigma\to\rho}. \quad \text{(additivity)} \\ \Rightarrow I_{\sigma\to\rho} &\leq I_\infty(\sigma) - I_\infty(\rho), \\ &= \log(\zeta_1 n) - \log(\eta_1 n), \\ &= \log\left(\frac{\zeta_1}{\eta_1}\right). \\ \Rightarrow 2^{-I_{\sigma\to\rho}} &\geq \frac{\eta_1}{\zeta_1}, \\ &= \frac{V_1(\rho)}{V_1(\sigma)}, \\ &\geq p^*, \quad \text{(by definition)} \end{aligned}$$

as required. □

There is a particular case that is worth commenting. From Eq. (2.30) we can see that when $I_{\rho\to\sigma} = -I_{\sigma\to\rho} \equiv I$ (that is, a transition that is reversible in the sense that the amount of work that is needed to perform it can be extracted in the opposite way) then $p^* = 2^{-I}$. This occurs when either $\sigma \overset{\text{NO}}{=} \rho \otimes s_{|I|}$ or $\rho \overset{\text{NO}}{=} \sigma \otimes s_{|I|}$ depending on whether $I$ is positive or negative (when

$I \geq 0$ the transition is deterministic). In terms of Lorenz curves, this means that the curves of $\rho$ and $\sigma$ have the same shape up to re-scaling by a factor $2^{-I}$. For example, this is the case when both $\rho$ and $\sigma$ are sharp states, and both Lorenz curves are straight lines.

As a final comment, the result above can be applied in the thermodynamic regime of many independent copies. If we want to perform a transition such as:

$$\rho^{\otimes N} \to \sigma^{\otimes N}, \tag{2.34}$$

we need an amount of work given by $-NI_{\rho\to\sigma}$. Hence, the probability of success in such a case is bounded by:

$$2^{NI_{\rho\to\sigma}} \leq p^* \leq 2^{-NI_{\sigma\to\rho}}, \tag{2.35}$$

which tends to 0 for large $N$. This can be seen as a naive way in which in the thermodynamic limit, in which systems have a big number of components, statistical fluctuations are suppressed.

### Lorenz curve interpretation

Something remarkable, hinted by the graphic way in which the work and the maximum probability of transition are defined, is that Theorem 8 can be thought of in very geometrical terms, as a general feature of convex curves.

In terms of the Lorenz curves, adding $I_{\rho\to\sigma}$ nonuniformity to $\rho$ to make the transition possible is equivalent to compressing the Lorenz curve with respect to the $x$-axis by a ratio $2^{-I_{\rho\to\sigma}}$, such that the curve of $\rho$ lies just above and touches that of $\sigma$. Hence, a compression by $p^* \geq 2^{-I_{\rho\to\sigma}}$ must mean that there is at least a point of the compressed curve just below or touching $\sigma$. A proof of this is given in Figure 2.2.

Extracting $I_{\sigma\to\rho}$ nonuniformity from $\sigma$ before performing NO into $\rho$ is equivalent to compressing the curve of $\rho$ by a ratio of $2^{-I_{\sigma\to\rho}}$ such that the curve of $\sigma$ lies just above and touches that of $\rho$. Hence, to prove the upper bound in Eq. (2.30), it suffices to show that in compressing the curve of $\rho$ by $p^*$ at least one point of the new curve must lie above or touch that of $\sigma$. In Figure 2.3 we show a diagrammatic version of the proof given in Section 2.1.2.

We stress something that will be used later in the case of thermal operations, that with Theorem 8 we are proving a general statement about convex curves. This is, that the minimum

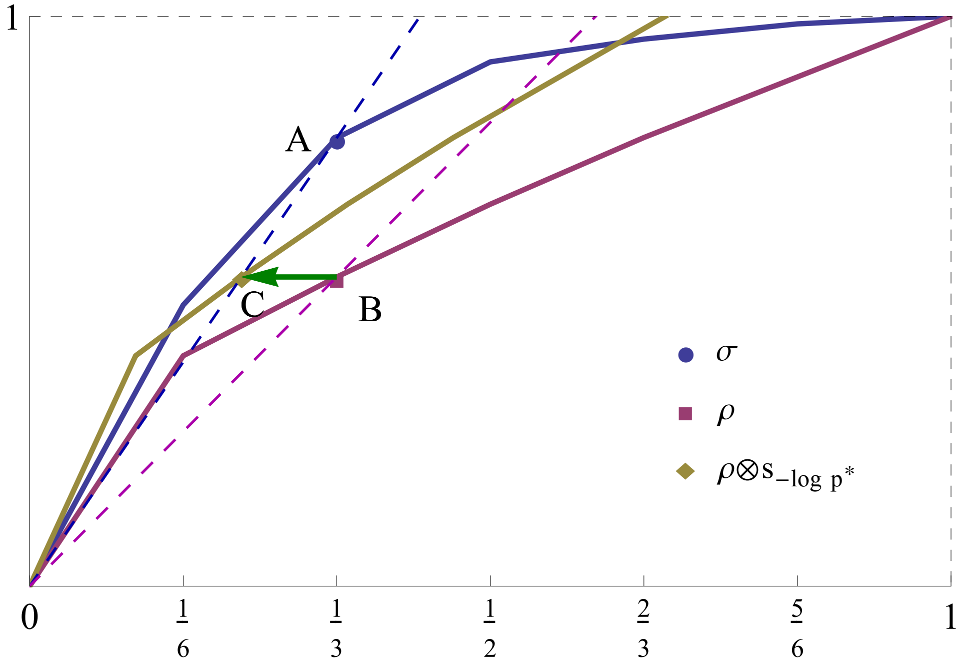

Figure 2.2: We plot the curves of $\rho$, $\sigma$ and $\rho$ compressed by a factor of $p^*$ with respect to the $x$-axis. The points $A$ and $B$ are those at which the vertical ratio between the curves of $\rho$ and $\sigma$ is maximum (which sets $l_1$ and $p^*$), and the sharp states that pass through those points are also shown as dashed lines. After compressing the Lorenz curve of $\rho$ by a ratio of $p^*$, the point $B$ will be taken to $C$, which will always either be below the curve of $\sigma$ or just touching it. This is equivalent to the lower bound in Eq. (2.30).

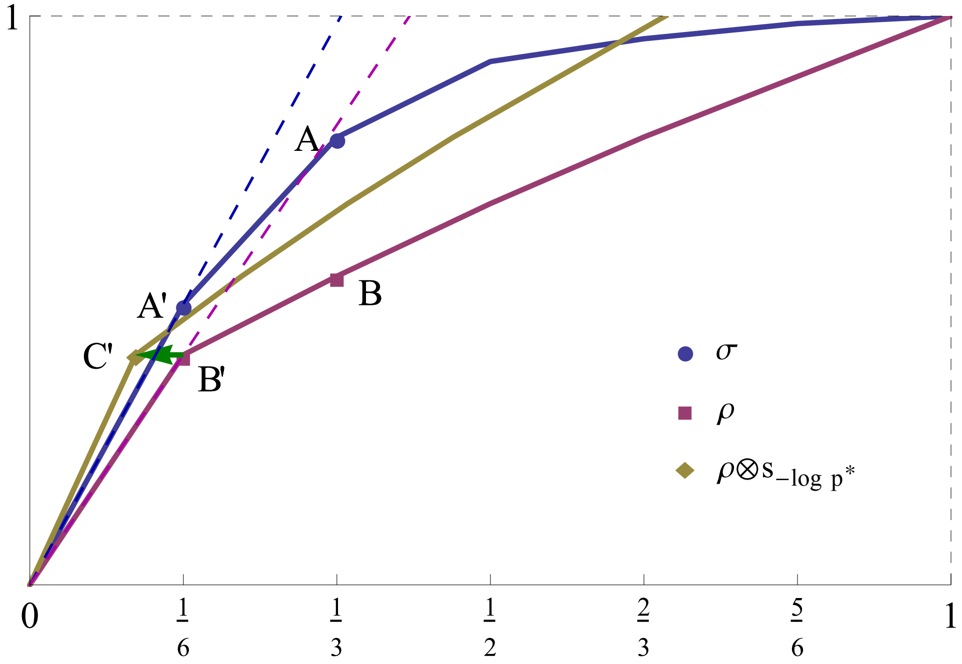

Figure 2.3: We plot the curves of $\rho$, $\sigma$ and $\rho$ compressed by $p^*$ (with respect to the $x$-axis). The points $A$ and $B$ at which the vertical ratio between the curves of $\rho$ and $\sigma$ is maximum (which sets $l_1$ and $p^*$) and the sharp states $I_\infty(\rho)$ and $I_\infty(\sigma)$ are also shown as dashed lines. Given that for sharp states all bounds are saturated, the appropriate maximum vertical and horizontal ratios coincide, and are $\eta_1/\zeta_1$, the ratio of the heights of $B'$ and $A'$. But this ratio is, by definition, bigger than or equal to $p^*$, the ratio between $A$ and $B$. This means that if the curve of $\rho$ is compressed by $p^*$, the point $B'$ is mapped to $C$ just above or touching the curve of $\sigma$. This is equivalent to the upper bound of Eq. (2.30).

vertical ratio of two given curves ($p^*$) is lower and upper bounded respectively by the minimum and the maximum horizontal ratio of the two.

## 2.2 Probability of transition under thermal operations

We now proceed to extend the results from the previous section to the more general context of thermal operations.

First, let us recall the thermomajorization diagrams, for which we plot the points:

$$\left\{\left(\sum_{i=1}^{k} e^{-\beta E_i^{(\rho)}}, \sum_{i=1}^{k} p_i^{(\rho)}\right)\right\}_{k=1}^{n}, \tag{2.36}$$

where now the superscript $\rho$ on $E_i$ and $p_i$ indicates that they have been $\beta$-ordered and this ordering depends on $\rho$. Thermo-majorization states that $\rho$ can be deterministically converted into a quasiclassical $\sigma$ if and only if its thermo-majorization curve never lies below that of $\sigma$, as is shown in Figure 1.5. In what follows, we assume that the $p_i$ have been $\beta$-ordered unless it is stated otherwise.

Similarly to how Eq. (2.3) defines monotones for the resource theory of noisy operations, the height of the $\beta$-ordered thermo-majorization curves provides monotones for Thermal Operations. If we denote the height of the thermo-majorization curve of $\rho$ at $x$ by $\tilde{V}_x(\rho)$, for $0 \leq x \leq Z$ (where $Z$ is the partition function), then by the thermo-majorization criteria, this function is non-increasing under thermal operations. In particular, for quasiclassical $\rho$, we have the following vertical monotones, analogous to those in Eq. (2.3) for noisy operations:

$$\tilde{V}_{x_k}(\rho) = \sum_{i=1}^{k} p_i^{(\rho)}, \quad \text{where } x_k = \sum_{i=1}^{k} e^{-\beta E_i^{(\rho)}}. \tag{2.37}$$

These monotones also give us an alternative way of stating the thermo-majorization criteria. In addition to the results shown in the previous chapter, we also show that the points to be checked at the curves are only those of the set $\mathcal{L}(\sigma)$, which are the horizontal positions of the elbows of the target state $\sigma$. This is related to what we showed for the work of transition in Lemma 5.

**Theorem 9.** *Suppose $\rho$ and $\sigma$ are quasiclassical states. Let $\mathcal{L}(\sigma) = \left\{\sum_{i=1}^{k} e^{-\beta E_i^{(\sigma)}}\right\}_{k=1}^{n}$. Then*

*$\rho$ can be deterministically converted into $\sigma$ under thermal operations if and only if:*

$$\tilde{V}_x(\rho) \geq \tilde{V}_x(\sigma), \quad \forall x \in \mathcal{L}(\sigma). \tag{2.38}$$

*Proof.* To prove this theorem, we make use of the concavity properties of thermo-majorization curves. Suppose $\rho \xrightarrow{TO} \sigma$. Then by thermo-majorization, $\tilde{V}_x(\rho) \geq \tilde{V}_x(\sigma)$, for $0 \leq x \leq Z$ and in particular Eq. (2.38) holds.

Conversely, suppose Eq. (2.38) holds and, setting $t_0 = 0$, label the elements of $\mathcal{L}(\sigma)$ arranged in increasing order by $t_i$ for $i = 1$ to $n$. Then on the interval $[t_{i-1}, t_i]$, for $1 \leq i \leq n$, the thermo-majorization curve of $\sigma$ is given by a straight line. From $\rho$, define the block-diagonal state $\rho_\sigma$ by the thermo-majorization curve:

$$\left\{\left(t_i, \tilde{V}_{t_i}(\rho)\right)\right\}_{i=1}^{n}, \tag{2.39}$$

and note that due to the concavity of thermo-majorization curves, $\rho$ thermo-majorizes $\rho_\sigma$. On the interval $[t_{i-1}, t_i]$, $1 \leq i \leq n$, the thermo-majorization curve of $\rho_\sigma$ is also given by a straight line. The construction of this state $\rho_\sigma$ is shown in Figure 2.4. We note this curve represents the state with the same $\beta$-order as $\sigma$ that is the most resourceful that can be reached from $\rho$, as it just touches the diagram of $\rho$ from below.

As $\tilde{V}_{t_i}(\rho_\sigma) = \tilde{V}_{t_i}(\rho)$, $\forall i$ by construction, Eq. (2.38) implies that $\tilde{V}_{t_i}(\rho_\sigma) \geq \tilde{V}_{t_i}(\sigma)$, $\forall i$. Hence on the interval $[t_{i-1}, t_i]$, $1 \leq i \leq n$, the thermo-majorization curves for $\rho_\sigma$ and $\sigma$, and therefore $\rho$ and $\sigma$, do not cross. As this holds for all $i$ and the intervals cover $[0, Z]$ the thermo-majorization curve of $\rho$ is never below that of $\sigma$ and we can perform $\rho \xrightarrow{TO} \sigma$ deterministically. □

If we define the number of 'elbows' in the thermo-majorization curve of $\sigma$ to be $j$, this reduces thermo-majorization to checking $j$ points and generalizes Lemma 17 of [80] to thermal operations.

### 2.2.1 Non-deterministic transformations

Having defined the appropriate monotones for thermal operations, and the appropriate way of phrasing the thermomajorization criteria, we are now in a position to investigate non-deterministic transformations and prove a theorem analogous to Theorem 7.

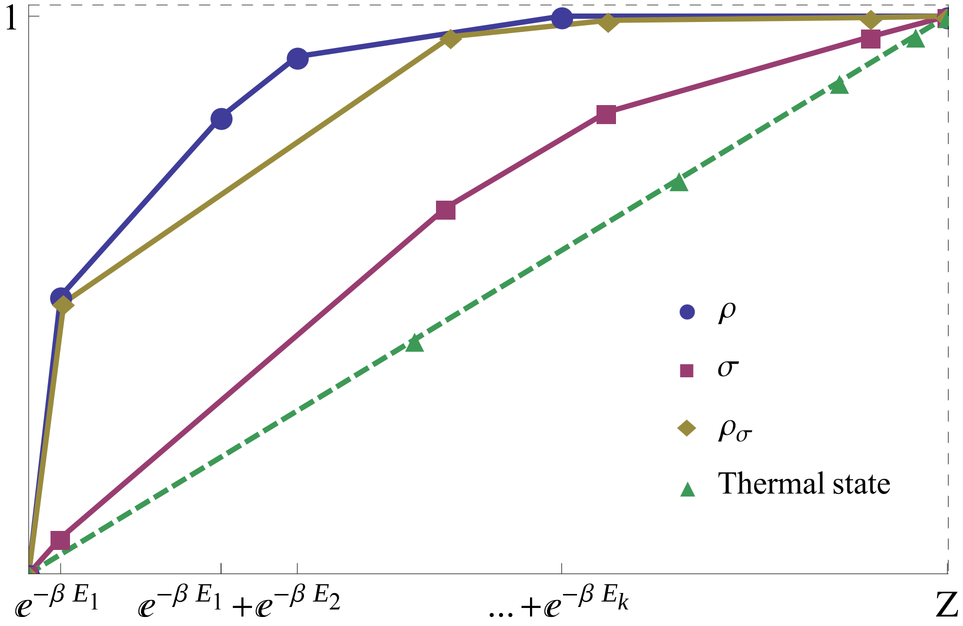

Figure 2.4: Here we illustrate the construction of the state $\rho_\sigma$ used in the proof of Theorem 9. The points of the curve $\rho$ are at the same horizontal position as the elbows of $\sigma$, and hence both states have the same $\beta$-order. By the concavity of the curves, the resultant curve of $\rho_\sigma$ is always below that of $\rho$.

**Theorem 10.** *Suppose we wish to transform the quasiclassical state $\rho$ to the quasiclassical state $\sigma$ under thermal operations. The maximum value of $p$, $p^*$, that can be achieved in the transition:*

$$\rho \xrightarrow{TO} \rho' = p\sigma + (1-p)\,X, \tag{2.40}$$

*is such that:*

$$p^* = \min_{x\in\mathcal{L}(\sigma)} \frac{\tilde{V}_x(\rho)}{\tilde{V}_x(\sigma)}. \tag{2.41}$$

*Proof.* Proving this result has additional complications with respect to the analogue of noisy operations Theorem 7. This is due to the fact that $\rho$ and $\sigma$ may have different $\beta$-orderings. Other than that, the structure of the proof will be as before. First we show that the quantity in Eq. (2.41) is an upper bound, and then we shall give a protocol that achieves it.

We prove the bound in Eq. (2.41) by constructing useful intermediate curves between those of $\rho$ and $p\sigma$ to deal with differing $\beta$-orders. With these in place, the result will follow in a similar manner to Theorem 7.

We begin by showing that given Eq. (2.40):

$$\tilde{V}_x(\rho) \geq p\tilde{V}_x(\sigma), \quad \forall x \in [0, Z]. \tag{2.42}$$

First consider the maximum value of $p$ that can be achieved in attempting to convert $\rho$ into $\sigma$

$$\rho \quad \overset{TO}{\longrightarrow} \quad \rho' \ = p\sigma + (1-p)\,X.$$

Again using Weyl's inequality as per Theorem 7 to deal with the potential coherences within degenerate energy levels, for $\rho'$, $\sigma$ and $X$, we have:

$$p_i' \geq pq_i, \quad \forall i, \tag{2.43}$$

where $p_i'$ and $q_i$ are the populations of $\rho'$ and $\sigma$ respectively. Now consider the sub-normalized thermo-majorization curve of $p\sigma$ given by the points:

$$\left\{\left(\sum_{i=1}^{k} e^{-\beta E_i^{(\sigma)}}, p\sum_{i=1}^{k} q_i^{(\sigma)}\right)\right\}_{k=1}^{n}, \tag{2.44}$$

and the (possibly non-concave) curve formed by plotting the eigenvalues of $\rho'$ according to the $\beta$-ordering of $\sigma$. This is given by the points:

$$\left\{\left(\sum_{i=1}^{k} e^{-\beta E_i^{(\sigma)}}, \sum_{i=1}^{k} p_i'^{(\sigma)}\right)\right\}_{k=1}^{n}, \tag{2.45}$$

where we remind that the superscript $(\sigma)$ indicates that the diagram has the $\beta$-order of $\sigma$. It is easy to see by Eq. (2.43) that the curve defined in Eq. (2.45) is never below that defined in Eq. (2.44).

Finally, the thermo-majorization curve of $\rho'$ is given by:

$$\left\{\left(\sum_{i=1}^{k} e^{-\beta E_i^{(\rho')}}, \sum_{i=1}^{k} \eta_i'^{(\rho')}\right)\right\}_{k=1}^{n}. \tag{2.46}$$

Note that attempting to construct a thermo-majorization curve for $\rho'$ with respect to the $\beta$-ordering of another state, as we do in Eq. (2.45), has the effect of rearranging the straight segments of the actual thermo-majorization curve. This means that they may no longer be joined from left to right in order of decreasing gradient. Such a curve will always be below the true thermo-majorization curve. To see this, imagine constructing a curve from the straight segments and in particular, trying to construct a curve that would lie above all other possible constructions. Starting at the origin, we are forced to choose the element with the steepest gradient - all other choices would lie below this by virtue of having a shallower gradient. We then proceed iteratively, starting from the endpoint of the previous section added and choosing the element with the largest gradient from the remaining linear segments. The construction that we obtain is the true thermo-majorization curve. A graphical description of this proof is shown in Fig. 2.5, where an example of all the curves considered is included.

We see then that the curve in Eq. (2.46) is never below that in Eq. (2.45). This gives us:

$$\tilde{V}_x(\rho) \geq \tilde{V}_x(\rho') \geq p\tilde{V}_x(\sigma), \tag{2.47}$$

where the first inequality holds as, by definition, $\rho$ thermo-majorizes $\rho'$. Rearranging and keeping just the tightest constraint, we have that:

$$p^* \leq \min_{x\in\mathcal{L}(\sigma)} \frac{\tilde{V}_x(\rho)}{\tilde{V}_x(\sigma)}. \tag{2.48}$$

A protocol that saturates the bound is:

$$\begin{aligned} \rho &\xrightarrow{TO} \rho_\sigma, \\ &\xrightarrow{TO} \rho'_\sigma = p^*\sigma + (1-p^*)X, \end{aligned}$$

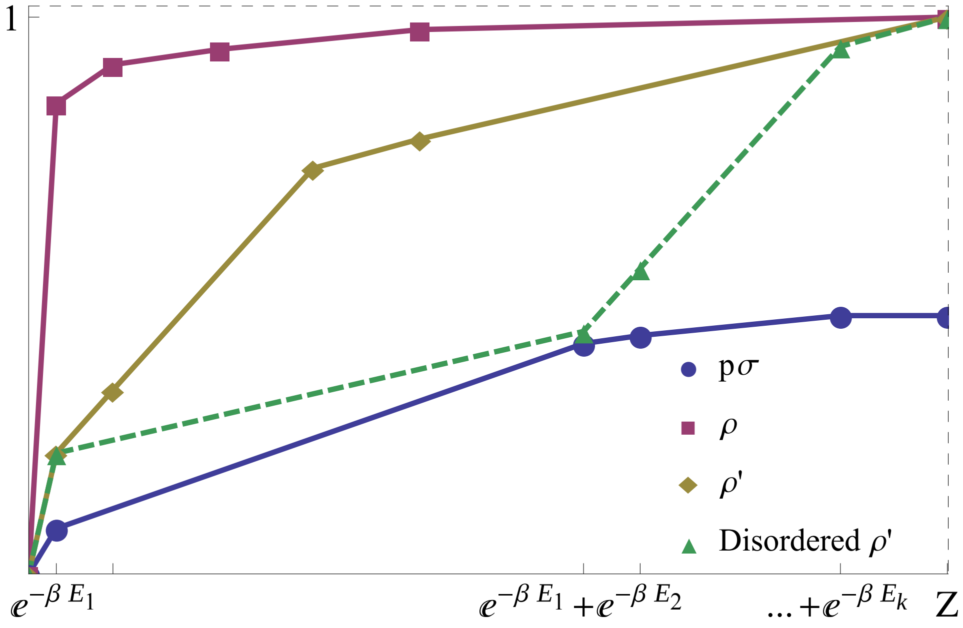

Figure 2.5: Here we show graphically the steps of the proof of the first part of Theorem 10. In the decomposition of Eq. (2.40) the curve $p\sigma$ must always be below that of $\rho'$ and hence also $\rho$. This sets the maximum probability $p^*$ as defined in Eq. (2.41). Both $p\sigma$ and the disordered $\rho'$ have the same $\beta$-ordering.

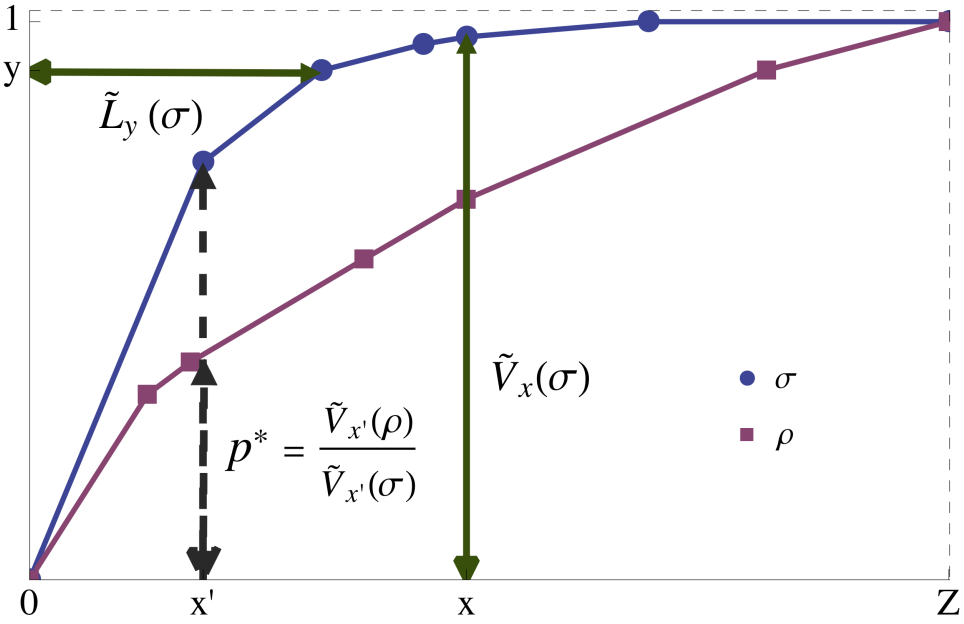

Figure 2.6: Here we show a pair of thermomajorization diagrams, and arrows shoing the magnitude of a horizontal monotone $\tilde{L}_y(\sigma)$ and a vertical one $\tilde{V}_x(\sigma)$. We show how the magnitude of $p^*$, the maximum probability for the transition $\rho \to \sigma$, is computed as the minimal ratio of two vertical monotones at position $x'$ in the diagram.

where $\rho_\sigma$ was defined in Eq. (2.39) and is thermo-majorized by $\rho$. As $\rho_\sigma$ and $\sigma$ have the same $\beta$-ordering and, by definition

$$\frac{\tilde{V}_x(\rho)}{\tilde{V}_x(\sigma)} = \frac{\tilde{V}_x(\rho_\sigma)}{\tilde{V}_x(\sigma)}, \quad \forall x \in \mathcal{L}(\sigma). \tag{2.49}$$

Hence we have a state $\rho_\sigma$ that has the same $\beta$-order as $\sigma$ and yet still Eq.(2.49) holds. This way we overcome the difficulty of having different $\beta$-order, and we can apply the same construction used in Theorem 7, which gives a strategy to produce $\rho'_\sigma$ that achieves:

$$p^* = \min_{x \in \mathcal{L}(\sigma)} \frac{\tilde{V}_x(\rho)}{\tilde{V}_x(\sigma)}. \tag{2.50}$$

□

We show an example of how we compute this ratio of monotones with the curves, as well as an illustration of both the horizontal and vertical monotones, in Fig. 2.6.

### 2.2.2 Bounds on the probability

The next important result of this chapter is the analogous of Eq. (2.30) for the thermal case, giving an upper and lower bound to the maximum probability for a transition:

**Theorem 11.** *Given two states* $\rho$ *and* $\sigma$*, where* $\sigma$ *is block-diagonal in the energy eigenbasis, under thermal operations:*

$$e^{\beta W_{\rho\to\sigma}} \leq p^* \leq e^{-\beta W_{\sigma\to\rho}}, \tag{2.51}$$

*where as* $p^* \leq 1$*, we assume* $W_{\rho\to\sigma} \leq 0$*. If* $W_{\rho\to\sigma} \geq 0$*,* $p^* = 1$ *and the transformation from* $\rho$ *to* $\sigma$ *can be done deterministically, potentially extracting a finite amount of work.*

*Proof.* The previous Theorem 8 can be seen as a general statement about pairs of concave Lorenz-like curves: the minimum vertical ratio is lower and upper bounded by the minimum and maximum horizontal ratios of the two. Given our previous definitions of the work of transition, and the fact that $p^*$ is the minimum vertical ratio of the two Lorenz curves (as shown in Theorem 10), the result follows.

□

In Section 3.4.2 in Chapter 3 we show how the upper bound of this theorem can be seen as a consequence of the Jarzynski equality.

This will come from the following intuition: the upper bound tells us that a transition from which work can be extracted (that is, $\sigma \to \rho$) cannot happen very often, as this would violate the second law. Equally, the value of that work extracted with probability $p^*$ cannot be very high.

### 2.2.3 Measuring whether the transition occurred under thermal operations

After obtaining $\rho'$ through thermal operations we may apply the measurement defined by Eq. (2.21) to extract our target state with probability $p^*$. In order to properly account for the cost of this measurement we now show how one can actually implement it.

A way to do it is through a process that uses an ancilla qubit system, $Q$, that starts and ends in the state $|0\rangle$ and has associated Hamiltonian, $H_Q = \mathbb{I}_2$, a unitary that correlates the system with the ancilla and a projective measurement on the ancilla qubit. As the measurement operators are diagonal in the energy eigenbasis, we will find that the unitary is energy conserving and within the set of thermal operations. Furthermore, the ancilla that is used to perform the POVM can be returned back into it's original state. Hence the only cost we have to pay is to erase the record of the measurement outcome itself. As is well known since the work of Landauer and Bennet [107, 21], the cost of erasing a binary record is $kT\log 2$. Although if one is repeating the process many times and is allowed to collectively erase the records, through data compression one can reduce the cost down to $kTh\left(p^*\right)$ with $h\left(p^*\right)$ the binary entropy $h\left(p^*\right) = -p^*\log p^* - \left(1-p^*\right)\log\left(1-p^*\right)$ [162]. This cost is the lowest such that the 2nd law is not broken on average.

The unitary that we shall use is given by:

$$U_{\mathrm{SQ}} = \begin{pmatrix} \sqrt{M} & \sqrt{\mathbb{I}-M} \\ \sqrt{\mathbb{I}-M} & -\sqrt{M} \end{pmatrix}, \tag{2.52}$$

where $M$ is defined as per Eq. (2.21). Note that it is also Hermitian $U_{\mathrm{SQ}} = U_{\mathrm{SQ}}^{\dagger}$. Its effect on the initial joint state is:

$$\begin{aligned}
&U_{\mathrm{SQ}}(\rho' \otimes |0\rangle\langle 0|)U_{\mathrm{SQ}}^{\dagger},\\
=&\begin{pmatrix} \sqrt{M} & \sqrt{\mathbb{I}-M} \\ \sqrt{\mathbb{I}-M} & -\sqrt{M} \end{pmatrix}\begin{pmatrix} \rho' & 0 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} \sqrt{M} & \sqrt{\mathbb{I}-M} \\ \sqrt{\mathbb{I}-M} & -\sqrt{M} \end{pmatrix},\\
=&\begin{pmatrix} \sqrt{M}\rho'\sqrt{M} & \sqrt{M}\rho'\sqrt{\mathbb{I}-M} \\ \sqrt{\mathbb{I}-M}\rho'\sqrt{M} & \sqrt{\mathbb{I}-M}\rho'\sqrt{\mathbb{I}-M} \end{pmatrix},\\
=&\begin{pmatrix} p^*\sigma & \sqrt{M}\rho'\sqrt{\mathbb{I}-M} \\ \sqrt{\mathbb{I}-M}\rho'\sqrt{M} & (1-p^*)X \end{pmatrix}.
\end{aligned}$$

If we now measure the ancilla in the computational basis, the joint state will collapse to $\sigma\otimes|0\rangle\langle 0|$ when the 0 outcome is observed. This happens with probability $p^*$. If the 1 outcome is observed, the joint state collapses to $X\otimes|1\rangle\langle 1|$ and this happens with probability $1-p^*$. In addition, if the 1 outcome is observed, we can then apply a Pauli $Z$ to the ancilla qubit to return it to its initial state.

To see that $U_{SQ}$ commutes with the total Hamiltonian and belongs to the class of thermal operations, first note that the total Hamiltonian is given by:

$$H_{SQ} = H_S \otimes \mathbb{I}_2 + \mathbb{I}_n \otimes \mathbb{I}_2. \tag{2.53}$$

The unitary trivially commutes with the second term so focusing on the first term, and noting that $M$ and $H_S$ are both diagonal matrices so commute, it is easy to check that:

$$\begin{aligned}[U_{\mathrm{SQ}}, H_S \otimes \mathbb{I}_2] = & \begin{pmatrix} \sqrt{M} & \sqrt{\mathbb{I}-M} \\ \sqrt{\mathbb{I}-M} & -\sqrt{M} \end{pmatrix} \begin{pmatrix} H_{\mathrm{S}} & 0 \\ 0 & H_{\mathrm{S}} \end{pmatrix} \\ & - \begin{pmatrix} H_{\mathrm{S}} & 0 \\ 0 & H_{\mathrm{S}} \end{pmatrix} \begin{pmatrix} \sqrt{M} & \sqrt{\mathbb{I}-M} \\ \sqrt{\mathbb{I}-M} & -\sqrt{M} \end{pmatrix}, \\ = & \, 0. \end{aligned}$$

Hence $[U_{SQ}, H_{SQ}] = 0$.

Observe that, although it is not necessary for our proof, this reasoning can be generalized to measurements with $s$ outcomes [130]. Provided the measurement operators commute with $H_S$, the measurement can be performed using a $s$-level ancilla system with trivial Hamiltonian and a joint energy-conserving unitary. Such a measurement can be performed for free up to having to spend work to erase the record of the measurement outcome at a cost of $kT \ln s$.

## 2.3 Heralded probability

Throughout the present chapter we have been considering the optimization of $p$ in the process:

$$\rho \xrightarrow{TO} \rho' = p\sigma + (1-p)\, X, \tag{2.54}$$

for given $\rho$ and $\sigma$. Another related notion of a probabilistic transformation one can think of is that of *heralded probability*, i.e. a conclusive fluctuation to a state. In this setup, a qubit flag system with trivial Hamiltonian $H_F \propto \mathbb{I}$ is incorporated from the start in the state $|0\rangle$ and after the thermal operation, indicates whether the system was successfully transformed into $\sigma$. More concretely, with respect to heralded probability and for given $\rho$ and $\sigma$ one would attempt to maximize $p$ in the process:

$$\rho \otimes |0\rangle\langle 0| \xrightarrow{TO} \hat{\rho} = p\sigma \otimes |0\rangle\langle 0| + (1-p)\, X \otimes |1\rangle\langle 1|, \tag{2.55}$$

where the total Hamiltonian is $H = H_S + H_F$. A measurement on the flag will result in the system being in state $\sigma$ with probability $p$ and state $X$ with probability $1-p$.

When $\sigma$ is block-diagonal in the energy eigenbasis, the measurement strategy given in Section 2.2.3 can be used to convert a protocol obtaining a value of $p$ in Eq. (2.54) into one that obtains a value of $p$ in Eq. (2.55). Indeed, it has been shown that the maximum value of $p$ that can be achieved in both scenarios for such $\sigma$ is identical [147].

However, analyzing the optimization of $p$ in Eq. (2.55) may be more tractable than the equivalent problem with respect to Eq. (2.54) as for the problem of heralded probability we may always take $X = \tau_S$, the thermal state of the system. To see this, assume that we start with the state-Hamiltonian pair:

$$\left(p\sigma \otimes |0\rangle\langle 0| + (1-p)\, X \otimes |1\rangle\langle 1|, H_S + H_F\right), \tag{2.56}$$

and then apply the following thermal operations:

1. Append a thermal state with Hamiltonian $H_B = H_S$:

$$\begin{aligned}&\left(p\sigma \otimes |0\rangle\langle 0| + (1-p)\, X \otimes |1\rangle\langle 1|, H_S + H_F\right)\\ \xrightarrow{TO}\, &\left(p\sigma \otimes \tau_B \otimes |0\rangle\langle 0| + (1-p)\, X \otimes \tau_B \otimes |1\rangle\langle 1|, H_S + H_B + H_F\right).\end{aligned}$$

2. Apply the unitary $U = \mathbb{I}_{SB} \otimes |0\rangle\langle 0| + U_{SB}^{swap} \otimes |1\rangle\langle 1|$ where $U_{SB}^{swap}$ is the unitary that swaps the state of the system with the state of the bath. As $H_S = H_B$, $[U, H_S + H_B + H_F] = 0$ and hence $U$ is a valid thermal operation. This implements:

$$\begin{aligned}&\left(p\sigma \otimes \tau_B \otimes |0\rangle\langle 0| + (1-p)\, X \otimes \tau_B \otimes |1\rangle\langle 1|, H_S + H_B + H_F\right)\\ \xrightarrow{TO}\, &\left(p\sigma \otimes \tau_B \otimes |0\rangle\langle 0| + (1-p)\, \tau_S \otimes X \otimes |1\rangle\langle 1|, H_S + H_B + H_F\right).\end{aligned}$$

3. Discard the bath system:

$$\begin{aligned}&\left(p\sigma \otimes \tau_B \otimes |0\rangle\langle 0| + (1-p)\, \tau_S \otimes X \otimes |1\rangle\langle 1|, H_S + H_B + H_F\right)\\ \xrightarrow{TO}\, &\left(p\sigma \otimes |0\rangle\langle 0| + (1-p)\, \tau_S \otimes |1\rangle\langle 1|, H_S + H_F\right).\end{aligned}$$

Hence, given a state of the form $\hat{\rho}$, we can always find a thermal operation that converts $X$ into $\tau_S$. In attempting to maximize $p$ in Eq. (2.55) we can thus always assume that $X$ is the thermal state of the system. This simplification will enable us to prove additional bounds on the maximum value of the heralded probability, $\hat{p}$, for catalytic thermal operations (as described in Section 1.4.1) and the case where $\sigma$ contains coherences in energy (as described in Section 1.6).

### 2.3.1 Heralded probability with catalysts

In catalytic thermal operations, given $\rho$ and $\sigma$, we are interested in whether there exists a state $\sigma_C$ such that:

$$\rho \otimes \sigma_C \xrightarrow{TO} \sigma \otimes \sigma_C. \tag{2.57}$$

If such a $\sigma_C$ exists, we say it catalyzes the transformation and write $\rho \xrightarrow{CTO} \sigma$. Determining whether such an $\omega$ exists has resulted in a different set of thermodynamic constraints [28].

Recall the definition of the generalized free energies of $(\rho, H_S)$ by:

$$F_\alpha^\beta(\rho) = kTD_\alpha(\rho||\tau_S) - kT\log Z_S, \tag{2.58}$$

where again $D_\alpha$ are the Rényi divergences given by:

$$D_\alpha(\rho||\tau_S) = \frac{\operatorname{sgn}(\alpha)}{\alpha - 1}\log \operatorname{Tr}\left[\rho^\alpha \tau_S^{1-\alpha}\right], \tag{2.59}$$

with $\tau_S$ the thermal state of the system. Then for quasiclassical $\rho, \sigma$, $\rho \xrightarrow{CTO} \sigma$ if and only if $F_\alpha^\beta(\rho) \geq F_\alpha^\beta(\sigma)$, holds $\forall \alpha \geq 0$.

To optimize the heralded probability of a transformation from $\rho$ to $\sigma$ under catalytic thermal operations, we thus want to maximize the value of $p$ in $\hat{\rho} = p\sigma \otimes |0\rangle\langle 0| + (1-p)\tau_S \otimes |1\rangle\langle 1|$ subject to these free energy constraints applied to $\rho$ and $\hat{\rho}$. This gives us:

$$\hat{p} \leq \max\left\{p : D_\alpha\left(\rho_D \otimes |0\rangle\langle 0|\middle|\middle|\tau_S \otimes \mathbb{I}_2\right) \geq D_\alpha\left(p\sigma_D \otimes |0\rangle\langle 0| + (1-p)\tau_S \otimes |1\rangle\langle 1|\middle|\middle|\tau_S \otimes \mathbb{I}_2\right), \alpha \in [0,\infty]\right\}.$$

This bound on $\hat{p}$ is achievable as the constraints given by the Renyi divergences [28] imply there exists a $\sigma_C$ such that:

$$\rho \otimes |0\rangle\langle 0| \otimes \sigma_C \xrightarrow{TO} (\hat{p}\sigma \otimes |0\rangle\langle 0| + (1-\hat{p})\tau_S \otimes |1\rangle\langle 1|) \otimes \sigma_C. \tag{2.60}$$

### 2.3.2 Heralded probability for arbitrary quantum states

For states with coherences, necessary and sufficient conditions for which state transitions are possible are not known in general. However, there exists various different sets of necessary conditions that can be used to give upper bounds to the optimal probability of transition. We give the bounds for two such sets, one in terms of quantum Renyi divergences and a second one in terms of modes of coherence.

For a given state with coherences in energy, we define the *free coherence* of a state $\rho$ by:

$$A_{\alpha}\left(\rho\right)=S_{\alpha}\left(\rho||\Delta\rho\right), \tag{2.61}$$

where $S_{\alpha}$ are the quantum Rényi divergences given by:

$$S_{\alpha}\left(\rho||\Delta\rho\right)=\begin{cases}\frac{1}{\alpha-1}\log\mathrm{Tr}\left[\rho^{\alpha}\Delta\rho^{1-\alpha}\right], & \alpha\in[0,1),\\ \mathrm{Tr}\left[\rho\left(\log\rho-\log\Delta\rho\right)\right], & \alpha=1,\\ \frac{1}{\alpha-1}\log\mathrm{Tr}\left[\left(\Delta\rho^{\frac{1-\alpha}{2\alpha}}\rho\Delta\rho^{\frac{1-\alpha}{2\alpha}}\right)^{\alpha}\right], & \alpha>1,\end{cases} \tag{2.62}$$

It was shown in [115] that for general $\sigma$, $\rho\xrightarrow{TO}\sigma$ only if $A_{\alpha}\left(\rho\right)\geq A_{\alpha}\left(\sigma\right)$ for all $\alpha\geq 0$.

Using this we obtain the following bound on the maximum heralded probability of a transformation from $\rho$ to $\sigma$ under thermal operations:

$$\hat{p}\leq\max\left\{p:A_{\alpha}\left(\rho\otimes|0\rangle\langle 0|\right)\geq A_{\alpha}\left(p\sigma\otimes|0\rangle\langle 0|+\left(1-p\right)\tau_{S}\otimes|1\rangle\langle 1|\right),\quad\alpha\in[0,\infty]\right\}. \tag{2.63}$$

Alternatively, following [121], we can define necessary constraints in terms of modes of coherence. Given a state $\rho$, we can decompose it as a sum given by

$$\rho=\sum_{k}\rho_{(k)}, \tag{2.64}$$

where $\rho_{(k)}$ is such that

$$e^{-iH_{S}t}\rho_{(k)}e^{iH_{S}t}=e^{-ikt}\rho_{(k)}, \tag{2.65}$$

where the variable $k$ takes the values of all possible energy gaps of the Hamiltonian $H_S$, so that for some $l,m$ we have that $k=E_l-E_m$.

Because of the time-translation symmetry property of thermal operations defined in Lemma 2, we know that thermal operations map coherence modes of the initial state to coherence modes of the final state $\rho'$ only. More concretely, let $\mathcal{T}(\rho)$ be a quantum map generated through a set of thermal operations on the system, then

$$\mathcal{T}(\rho_{(k)})=\rho'_{(k)},\quad\forall k, \tag{2.66}$$

and hence, given that the 1-norm $||X||_1\equiv\mathrm{Tr}(\sqrt{XX^{\dagger}})$ is contractive under quantum maps, we have that $||\rho_{(k)}||_1\geq||\rho'_{(k)}||_1$ for all $k$.

This is used in [121] to show that, given a probabilistic transition of the form of

$$\rho \otimes |0\rangle\langle 0| \overset{TO}{\to} \left(p\sigma \otimes |0\rangle\langle 0| + (1-p)\, X \otimes |1\rangle\langle 1|, H_S + H_F\right), \tag{2.67}$$

where we may take the state $X$ to be thermal, we have a further set of necessary upper bounds on the maximum probability of transition, one for each $k$. The most constraining of them is then

$$p^* \leq \min_k \frac{||\rho_{(k)}||_1}{||\sigma_{(k)}||_1}. \tag{2.68}$$

## 2.4 Outlook

We here derived a fundamental limitation on probabilistic transitions via thermodynamical processes. A potentially useful generalization of this result is to derive the bounds for the probability to reach an ensemble of different states with different probabilities $\{\sigma_i, p_i\}$, perhaps involving a distribution of work, taking the result even closer to the realm of fluctuation theorems. A version of this question for the case of entanglement was answered in [98].

In the following chapter we will see how one of the bounds follows in certain cases from considering the Jarzynski equality. It would be interesting to know whether in the context of fluctuation relations we can see processes in which the maximum probability $p^*$ is actually reached or at least approximated, and whether these sort of transitions are special in some sense.

We have provided limitations imposed on probabilistic transitions involving quantum coherence. As a last remaining open question, one would like to derive not only limitations but achievable bounds, like the $p^*$ given here for quasiclassical states. Finding an expression for that maximum probability may be a step towards a sort of fully quantum fluctuation theorems. In any case, for that, first the necessary and sufficient conditions for transitions involving coherence have to be derived and, as we saw in Section 1.6, these are not yet known.

## 2.5 Summary

Starting from the results of Chapter 1, we here carried on exploring the power of the resource-theoretic framework by introducing and motivating a new kind of thermodynamical transition, the *probabilistic transition.* We show the fundamental limitation to probabilistic transitions by giving an expression for the maximum possible probability, and we relate it to the work of deterministic transitions. We also show how all these results have very simple interpretations in terms of thermo-majorization curves, which can be seen as an example of the power of such graphical description of states.

In the beginning of the chapter we introduced a simpler resource theory: that of noisy operations. The reason to do this was that some of the results were much easier to prove within it, and could then be used to prove the results in the more general thermal operations.

An important point in the discussion is the cost associated to verifying whether the right probabilistic transition has occurred. While this requires a measurement which is outside the class of allowed operations, we have shown how to explicitly account for it by implementing the measurement through a free operation in which a pure qubit is added as the resource.

In order to extend our framework and possible transitions, we introduced the notion of heralded transitions, in which a flag system is involved. Using this auxiliary system, one can derive bounds given the thermodynamic constraints that are relevant in the context of catalysis and coherence.

The form of the bounds relating the probability of a fluctuation between states and the work of transition hint at a possible connection with fluctuation theorems, which will be elaborated in the next chapter.

# Chapter 3

# Work fluctuations

In the previous chapters we have introduced and explored the notion of deterministic work as useful and ordered energy that can be extracted from quantum systems through thermal operations. This notion has some appealing properties, including a very intuitive meaning in terms of thermomajorization diagrams. It also fits the intuition from classical thermodynamics that work should be a very well ordered amount of energy, without stochastic fluctuations.

However, looking a bit more carefully at the non-equilibrium physics literature, one may soon realize that this idea is quite restrictive. In fact, the relevant notions of work that more often appear in experimental settings involving small or quantum systems generally exhibit stochastic fluctuations. That is, in many cases we want to talk about changes of energy that are not necessarily definite, but that still have some property that distinguishes them from the purely thermal ones (that is, heat). For example, one may look at the change of energy of a working body before and after a closed operation, and understand that as work. This is thus a quantity that may change in different individual runs of different experiments.

An important questions arises: if we give up the idea of work as a definite amount of energy, how should we exactly think of these fluctuations? More precisely, how can we tell the difference between work and heat?

We know that whichever our notion of work is, it must be such that it obeys some form of second law of thermodynamics. For instance, in the case of deterministic work we saw that we always require more of it to create a non-equilibrium state from a thermal one than the amount we can extract from it. In general, a second-law like constraint will take the form of a bound on how much work we can extract along a process, and for cyclical ones this should always be negative on average.

The notion of work as a fluctuating quantity gives room for the appearance of some of the most important relations of nonequilibrium statistical physics: the fluctuation theorems. The formulation of these goes back to the work of Evans et al. [65], Gallavotti and Cohen [72], and perhaps more importantly, to the seminal work of Jarzynski and Crooks in the late 90s [94, 46].

If we understand the second law as an inequality between thermodynamical quantities, fluctuation theorems can be seen as a very radical strengthening of such a relation. These theorems take the form of averages of exponentials of random variables of non-equilibrium processes. From them, inequality statements akin to the second law can be derived. Because of their form, however, they contain more information about the occurrence of non-equilibrium fluctuations, and in particular, they illustrate how individual events that "break" the second law happen only with exponentially low probability.

In this chapter we will review some of the better known formulations of different fluctuation theorems, and we will then describe in which way these can be included within the context of resource theories, mostly following [5]. First we proceed to briefly describe the fluctuation theorems of Jarzynski and Crooks for closed systems.

## 3.1 Fluctuation theorems

The literature on non-equilibrium fluctuation theorems is vast and growing, and finding the most general situation where one can be defined, or a full set of quantum processes obey one, is still an active topic of research, with recent theoretical advances being, for instance [155, 127, 139, 113], although perhaps the most notable progress in recent years has been on the experimental side [126, 19, 54, 15].

One of the most important integral fluctuation theorems, that of Jarzynski [94]. It reads

$$\langle e^{\beta w} \rangle = \frac{Z'_S}{Z_S}, \tag{3.1}$$

where $w$ is the work done by the system along a particular process in which a system is driven out of thermal equilibrium, and $Z_S, Z'_S$ are the partition functions at the beginning and at the end of the process.

On top of it we find Crooks theorem, which is a refinement of such a relation that is based on the definition of a *reversed process*, which will be an important notion throughout this section. One can think of a protocol that extracts an amount of work given by a probability distribution $p(w)$ via driving some state out of equilibrium. Then, a particular reversed protocol can be defined in which a probability distribution $p_{\mathrm{rev}}(-w)$ is extracted. Crooks theorem then states that these two are related by

$$\frac{p(w)}{p_{\mathrm{rev}}(-w)} = \frac{Z'_S}{Z_S} e^{-\beta w}. \tag{3.2}$$

That is, the probability of extracting work in the forward direction is exponentially suppressed with respect to the probability of extracting negative work in the reversed direction. Generally, the reversed protocol is defined as a path in the space of control parameters that comes from reversing exactly the path in that space corresponding to the forward process (note that this is not equivalent to reversing the system dynamics, which may be irreversible).

Different variations of this kind of fluctuation theorem have been derived in a variety of classical and quantum settings. To mention a few: closed systems [173], in the context of both weak and strongly coupled open systems [41, 42], or for general quantum maps [4, 118] . There are also fluctuation theorems not for just the work but for the entropy production [159], with modifications when feedback is included in the protocol (both classical [156] and quantum [129]). Perhaps the most careful account of fully quantum fluctuation theorems, where also the control parameters play an important role, can be found in [3]. See [40, 63] for general reviews on the subject.

We now show the simplest proof of a Crooks and Jarzynski relation for a closed quantum system, in which there is no bath and the work is accounted for via energy measurements, two limitations which will be overcome later on. This follows the original idea of Tasaki [173], and thus we will refer to it as either Crooks or Tasaki-Crooks theorem.

The protocol for the forward process will be:

- Prepare a system in its thermal state at temperature $\beta$, $\tau_\beta = \frac{e^{-\beta H_S}}{Z_S}$.
- Measure its energy and record the value $E_i$.
- Apply an arbitrary unitary $U$ (not necessarily energy conserving) that drives it out of thermal equilibrium to $U\tau_\beta U^\dagger$.

- Measure the energy again $E'_j$. We note that the Hamiltonian of the system may have changed along the unitary protocol into $H'_S$, by the ancilla-qubit mechanism of Section 1.5 or some other control protocol.

- Repeat many times and compute the work probability distribution $p(w)$. The work for a particular run is given by $w = E_i - E'_j$, the change of energy in the system caused by the unitary.

The backwards protocol can be thought of as the following

- Prepare a system in its thermal state at temperature $\beta$, $\tau'_\beta = \frac{e^{-\beta H'_S}}{Z'_S}$, where the Hamiltonian is now the Hamiltonian at the end of the forward protocol.

- Measure energy $E'_j$ again (note that it may be a different $j$ to the one obtained in the forward protocol).

- Apply the reversed protocol, which for simplicity we shall take to be that of applying $U^\dagger$, so that we obtain $U^\dagger \tau'_\beta U$.

- Measure the energy again (the Hamiltonian will be back to $H_S$) and compute the work statistics $p_{\text{rev}}(-w)$, where now $-w = E'_j - E_i$.

Now we show that Crooks theorem holds for this protocol.

**Theorem 12.** *The work distributions of the forwards and backwards processes obey the following relation*

$$\frac{p(w)}{p_{rev}(-w)} = e^{-\beta w}\frac{Z'_S}{Z_S} \tag{3.3}$$

*Proof.* The work distribution for the forward process can be written as

$$p(w) = \sum_{i,j} \delta(w - E_i + E'_j)\langle j|U|i\rangle\langle i|U^\dagger|j\rangle \frac{e^{-\beta E_i}}{Z_S}. \tag{3.4}$$

We can also write that of the backwards similarly, and with some algebra we arrive to the identity of Eq. (3.2).

$$
\begin{aligned}
p_{\text{rev}}(-w) &= \sum_{i,j} \delta(-w - E'_j + E_i)\langle i|U^\dagger|j\rangle\langle j|U|i\rangle \frac{e^{-\beta E'_j}}{Z'_S} && (3.5)\\
&= e^{\beta w} \sum_{i,j} e^{-\beta(E_i - E'_j)} \delta(-w - E'_j + E_i)\langle i|U^\dagger|j\rangle\langle j|U|i\rangle \frac{e^{-\beta E'_j}}{Z'_S} && (3.6)\\
&= e^{\beta w} \sum_{i,j} \delta(-w - E'_j + E_i)\langle j|U|i\rangle\langle i|U^\dagger|j\rangle \frac{e^{-\beta E_i}}{Z'_S} && (3.7)\\
&= e^{\beta w} p(w) \frac{Z_S}{Z'_S}. && (3.8)
\end{aligned}
$$

□

This is a particularly simple instance of Crooks theorem because of the way we have defined the backwards protocol: merely as that generated by $U^\dagger$. We stress that this definition is not the only possible one, and the same relation may hold for other reversed processes.

As a simple corollary we find Jarzynski's equality.

**Corollary 1.** *Jarzynski's equality Eq.* (3.1) *holds for both the forward and the backwards process.*

*Proof.* This follows straightforwardly from Crooks theorem, by taking the appropriate average of the exponential of the work. That is, we first rewrite it as

$$
p(w)e^{\beta w} = \frac{Z'_S}{Z_S} p_{\text{rev}}(-w), \tag{3.9}
$$

and then sum over $w$ to obtain

$$
\sum_w p(w)e^{\beta w} = \langle e^{\beta w}\rangle = \frac{Z'_S}{Z_S}. \tag{3.10}
$$

An analogous expression can be derived for $p_{\text{rev}}(-w)$. □

A common protocol is that in which the unitary is created via a driven change in the Hamiltonian $H_S(t)$ over some time interval $[0, \tau]$. That is

$$
U = \mathcal{T} e^{-i\int_0^\tau H_S(t)\mathrm{d}t}, \tag{3.11}
$$

where the $\mathcal{T}$ stands for the fact that the integration is *time-ordered.* This way, $H_S = H_S(0)$ and $H'_S = H_S(\tau)$. In that case, the reversed protocol can be defined as the unitary generated by the opposite driving, which is $H_S^{\text{rev}} = H_S(\tau - t)$, and the unitary is

$$U^{\text{rev}} = \mathcal{T} e^{-i \int_0^\tau H_S(\tau - t) \mathrm{d}t}. \tag{3.12}$$

This corresponds to the reversed path in the space of control parameters. It is easy to see that $U^\dagger = U^{\text{rev}}$ if $\forall t, t' \in [0, \tau]$, we have that $[H_S(t), H_S(t')] = 0$. That is, if the Hamiltonian commutes with itself at all times. This also implies that we can drop the time order $\mathcal{T}$ from the integration.

It can be shown that Crooks theorem in Eq. (3.2) still holds if we define the reversed process in the more general way given by Eq. (3.12). A proof of this is, involving concepts such as Fourier transforms and characteristic functions, is beyond the scope of this thesis, but we refer the reader to, for instance [40]. The concept of a characteristic function of work has been particularly studied in the past times, as it has been found that it can be measured with phase estimation techniques [59, 126, 19], which makes the computation of work distribution functions in quantum systems very tractable, and within current experimental capabilities [19].

We have shown that Crooks theorem applies to a system that is not in contact with the bath along the unitary process. However, the only requirement from the system was that it starts in the thermal state. This means that the result of Theorem 12 applies if we consider a bigger object which is a system and a bath together, such that they are both in a thermal state. In that case, we measure the energy of system and bath at the beginning and end of the protocol (the energy change in the bath can now be thought of as *heat*), and the difference will be the work of the protocol that obeys the fluctuation theorem. That is, instead of measuring just $E_i, E'_j$, we also measure the energy of the bath $Q_i, Q_j$, and the work will be defined as

$$w = E_i + Q_i - E'_j - Q_j. \tag{3.13}$$

This idea will be of relevance in the rest of the chapter, where we will show how can fluctuation theorems fit into the resource-theoretic setting. In doing that we will be considering fluctuation theorems in which the unitary is applied to system and bath together.

## 3.2 Fluctuating work in thermal operations

We have seen in the previous section that work was defined as the change of energy of the system when projective measurements are performed, that is, $w = E_i - E'_j$. Where does this energy come from or go to? The unitary of the process is not energy-conserving, so it will come from the particular physical object that implements and controls that unitary.

In the resource theory approach, however, we want to keep track of all sources of energy. That is the main theoretical reason for why we want to have a work storage system, or a battery: the global protocol has to be such that total energy conservation holds.

An example of such a battery was introduced in Section 1.1.3 in the context of deterministic work, where we imposed that it should be a definite amount of energy that is increased or decreased. How do we construct a battery that stores a mixture of work values? Evidently this will involve a battery with many energy levels, but then some complications arise. We do not want work to be *any* kind of energy change, but it should be constrained in some way.

For instance, if we have a battery in some low energy eigenstate, we could put it in contact with a heat bath and thermalize it, such that it absorbs energy. Such energy cannot be really counted as work, but as heat transferred from the bath. It seems then that in order to be able to identify energy changes in the battery as work we need to constrain the way it interacts with the bath.

A natural abstract way to do so is that of imposing that interactions with the battery need to be *translationally invariant*, such that the process is independent of where the battery is at the beginning of a particular process. This was, to the author's knowledge, first suggested in [162]. We will define it in the next section.

With this constraint we maintain part of the intuition coming from classical equilibrium thermodynamics: that work should be some energy that is stored or expended, no matter where the battery was initially. If one thinks of a classical weight in a uniform gravitational field (a common textbook illustration of classical macroscopic work), the amount of work we extract is independent of where this is initially.

We will impose this constraint on the way the thermal operations act on the battery, and find that this has a variety of desirable consequences.

### 3.2.1 Thermal operations with fluctuating work: definition and properties

In the present setting we include a system with Hamiltonian $H_S$, and a bath with Hamiltonian $H_B$ initially in the thermal state $\rho_B = \frac{1}{Z_B}\mathrm{e}^{-\beta H_B}$, in the same way as it was done before. The Hamiltonian of the system can change through the protocol with a mechanism analogous to that described in Section 1.5.

The extra ingredient now is that we will be including an ideal battery with Hamiltonian $H_W = \int_{\mathbb{R}} dx\, x |x\rangle\langle x|$, where the orthonormal basis $\{|x\rangle, \forall\, x \in \mathbb{R}\}$ represents the position of the battery. As before, any joint transformation of system, bath and battery is represented by a quantum map $\Gamma_{SBW}$. A diagram illustrating these operations is given in Fig. 3.1.

The thermal operations at hand must be such that again the following conditions are satisfied:

**Unitary on all systems** The map is unitary on the three components: $\Gamma_{SBW}(\rho_{SBW}) = U\rho_{SBW}U^\dagger$.

**Energy conservation** The unitary commutes with the total Hamiltonian: $[U, H_S + H_B + H_W] = 0$. If the Hamiltonian of the system changes, instead the condition is given by Eq. (1.93).

On top of that we add the extra constraint, which amounts to a definition of work in this setting. The constraint can be defined as

**Definition 13.** *[Independence of the "position" of the battery] The unitary commutes with the translations on the battery:* $[U, \Delta_W] = 0$.

*Here* $\Delta_W$ *is the generator of the translations in the battery and canonically conjugate to the position of the battery* $H_W$*, that is* $[\Delta_W, H_W] = i$.

In what follows, it is useful to denote the eigenvectors of the generator of the translations on the battery $\Delta_W = \int dt\, t\, |t\rangle\langle t|$ by $|t\rangle$. One can think of these eigenstates as the "momentum" eigenstates of the battery, which given the position dependence of the Hamiltonian of the battery, also act as "pointer states" if we understand our battery as a quantum clock. Hence in some way these eigenstates can be understood as representing time.

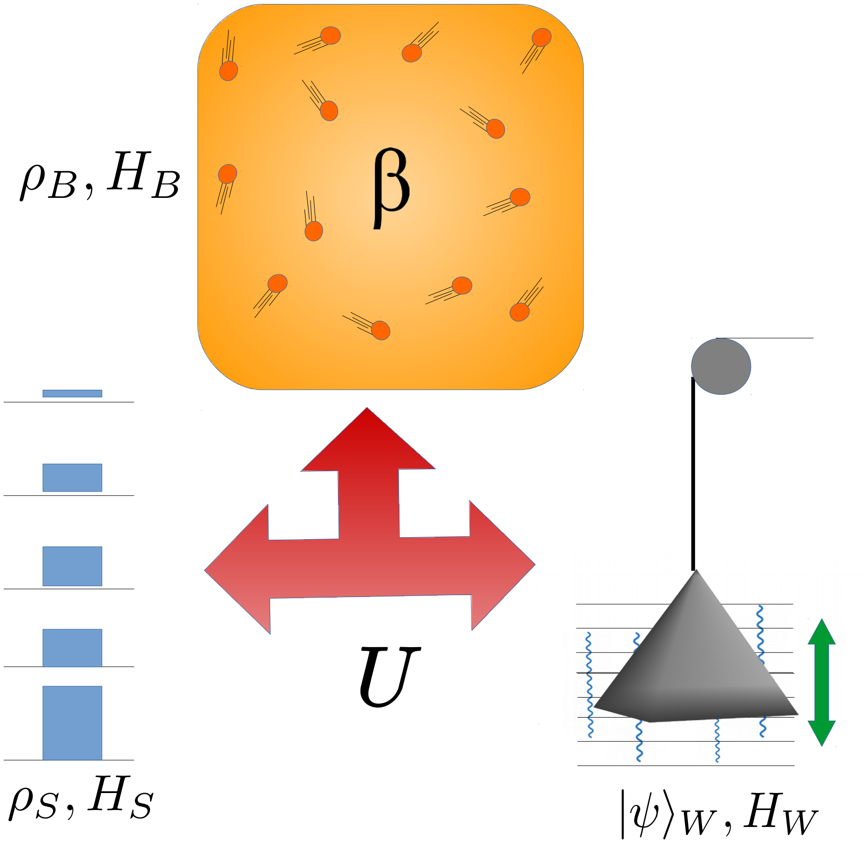

Figure 3.1: In thermal operations, a thermal bath interacts with a system with some populations in the energy eigenbasis, and with a quantum battery. The interaction between the three components is a global unitary that commutes with the sum of the three hamiltonians.

As a first desirable consequence, this condition implies that the reduced map on system and bath $\Gamma_{SB}$ is a mixture of unitaries. Hence the transformation can never decrease the entropy of system and bath, which guarantees that the battery is not used as a resource or as an entropy sink. This is guaranteed by the following lemma.

**Lemma 7.** *A map $\Gamma_{SBW}$ obeys the three constraints above (unitarity, energy conservation, and independence on the state of the battery) if and only if there is an arbitrary system-bath unitary $V_{SB}$ such that the global unitary on system, bath and battery can be written as*

$$\begin{aligned} U_{SBW} &= e^{i(H'_S+H_B)\otimes\Delta_W}\,(V_{SB}\otimes\mathbb{I}_W)\,e^{-i(H_S+H_B)\otimes\Delta_W} \\ &= \int dt\, A_{SB}(t)\otimes|t\rangle\langle t|\ , \end{aligned}$$

*where we define the family of unitaries*

$$A_{SB}(t) = e^{it(H'_S+H_B)}V_{SB}\,e^{-it(H_S+H_B)}\ .$$

*Proof.* The technical proof can be found in Lemma 13 in Appendix A.1. □

That the entropy of system-bath does not decrease follows as a corollary of Lemma 7.

**Corollary 2.** *The von Neumann entropy of system and bath does not decrease under thermal operations with translation invariance on the battery.*

*Proof.* Lemma 7 allows one to obtain an explicit form for the effective map on system-bath (after tracing out the battery)

$$\begin{aligned} \Gamma_{SB}(\rho_{SB}) &= \mathrm{tr}_W\Big(U_{SBW}\,\rho_{SB}\otimes\rho_W U^\dagger_{SBW}\Big) \\ &= \int dt\, A_{SB}(t)\rho_{SB}A^\dagger_{SB}(t)\,\langle t|\rho_W|t\rangle\ . \end{aligned} \tag{3.14}$$

By noting that $\langle t|\rho_W|t\rangle$ is a probability distribution, we see that the reduced map on system and bath $\Gamma_{SB}$ is a mixture of unitaries.

A mixture of unitaries is a unital operation that preserves the identity, so $\Gamma_{SB}(\mathbb{I}) = \mathbb{I}$. Therefore, the spectrum of the initial state majorizes that of the final state. This has as a particular consequence [80] that the von Neumann entropy $S(\rho) = -\mathrm{Tr}\rho\log\rho$ increases, so $S(\rho_{SB}) \le S(\Gamma_{SB}(\rho_{SB}))$.

□

This corollary implies that, even if the battery is for instance in a pure state, we are not using this purity as a thermodynamic resource, but we are only using it to store energy, which is what we truly want it for.

The condition of independence of the position of the battery can be thought of as a definition of work [162] and we show in the rest of the chapter how it is used in the appearance of fluctuation theorems within the resource-theoretic context.

In the case of Crooks theorem as shown in Theorem 12, one can argue that the assumption of a translation-invariant battery is implicit, since the amount of work is taken to be the difference in energy between the initial and final system/bath, and there is no explicit mention to the system that we need to include in order to make the global unitary energy-conserving.

We will see in the next sections how we can alternatively understand work as a change in energy of either the work system (explicit), or change in energy of the system-bath (implicit). In both cases work corresponds to a change in energy of the work system, and does not depend on how much energy is currently stored there. That comes from the fact that the global unitary commutes with the translation operation.

Next we discuss the connection between different paradigms in more detail and, in particular, show explicitly how within thermal operations the inclusion of such a translation invariant battery can help us include the Tasaki-Crooks fluctuation theorems for arbitrary unitaries.

### 3.2.2 Arbitrary unitaries and Tasaki-Crooks

We now show how the fluctuation theorems via arbitrary unitaries on the system can be obtained within the resource theory framework. Essentially what we want to show is which kind of battery state is needed in order to be able to implement an arbitrary unitary. We will be using the battery to apply the unitary, but the work random variable will still be defined through energy measurements on system and bath.

For this we take the state of the battery to have coherences over energy levels, which allows us to implement arbitrary unitaries on system and bath. Similar results are shown in [29, 2]. While this is a useful resource, the difficulty is that now we cannot measure the work random variable as an energy change of the battery, as the act of measuring would destroy the information in the coherences.

Theorem 1 extended to system and battery together implies that coherences in the battery are only needed if we wish to explicitly model a unitary which creates coherences over energy levels. These more general unitaries, however, are what is usually considered in the literature [40].

The key point is to note that Eq. (3.14) implies that, if the initial state of the battery $\rho_W$ is an eigenstate of $\Delta_W$, then the mixture of unitaries only has one term, so that

**Theorem 13.** *If the battery is in a maximally coherent state, that is, an eigenstate of* $\Delta_W$ *with eigenvalue* $t'$*, the effect on system and bath is an arbitrary unitary*

$$\Gamma_{SB}(\rho_{SB}) = A_{SB}(t')\rho_{SB}A_{SB}(t')^\dagger, \tag{3.15}$$

*where*

$$A_{SB}(t') = e^{it'(H'_S+H_B)}V_{SB}\, e^{-it'H_S+H_B)}, \tag{3.16}$$

*and* $V_{SB}$ *is as defined in Lemma 7.*

*Proof.* In the particular case where of Eq. (3.14) where $\rho_W = |t'\rangle\langle t'|$ is an eigenstate of of $\Delta_W$ so that $\Delta_W|t'\rangle = t'|t'\rangle$, the integral is then

$$\begin{aligned}\Gamma_{SB}(\rho_{SB}) &= \int dt\, A_{SB}(t)\rho_{SB}A^\dagger_{SB}(t)\,\delta(t-t') \\ &= A_{SB}(t')\rho_{SB}A_{SB}(t')^\dagger. \end{aligned}\tag{3.17}$$

□

That is, even though this effective map involves tracing out the battery, the result on system-bath is still unitary. This unitary is totally unconstrained, and in particular, it need not be energy-conserving. As pointed above, a typical form for this unitary is $\mathcal{T}\exp\left[-i\int dt\, H_{SB}(t)\right]$, where $\mathcal{T}$ is the time-order operator.

Given that in this way we have access to arbitrary unitaries, one can then derive the Tasaki-Crooks fluctuation theorems from Section 3.1.

In fact, we can derive something slightly more general. In the proof of Theorem 12 we only needed the fact that the unitary map is indeed unital. Hence, the two point measurement scheme gives a fluctuation theorem for any process on system and bath described by a unital map.

An important caveat of the results of this section is that they require the battery to be in a perfect coherent state $|t'\rangle$. While exactly attaining this state is physically impossible, arbitrarily good approximations are possible in principle, allowing for the implementation of maps arbitrarily close to unitary [2].

## 3.3 Quantum identities with an explicit battery

We have considered how one can use the battery to apply arbitrary unitaries on system and bath. Our next aim is to show how can it be used to actually store work, understood as an energy difference that we can measure after a protocol has taken place.

For this, we shall show that all the fluctuation theorems of the section come from a relation between the forward quantum channel on system and battery, and what we define as the backwards channel. We shall show that this relation is related to a concept that appears in quantum information theory called a *recovery map*, on which we will elaborate in Chapter 4.

Our notions of forwards and backwards will be the possibly simpler ones we can think of: if the forward is generated through a global unitary $U$, the backwards will be the thermal operation generated by unitary $U^\dagger$. Other more refined definitions of reversed processes can be found in [3], which involve constructions where all the control parameters are taken into account[1]. We however will not delve into this slightly subtle point, and just take the simple definition above.

We will be interested in the joint dynamics of system and battery, described by the quantum map

$$\Gamma_{SW}(\rho_{SW}) = \mathrm{tr}_B\left[U\left(\rho_{SW} \otimes \frac{e^{-\beta H_B}}{Z_B}\right)U^\dagger\right]. \tag{3.18}$$

The following definition will be useful, which as we will see can be thought of as a quantum generalization of the exponentials that appear in the fluctuation relations. A similar operator was previously used in [48].

**Definition 14.** *We define the following completely positive but not trace preserving map as*

---

[1] The idea there is that if one wants to switch between the dynamics of the forward and backwards processes one does so by switching certain control parameters that are part of the setting.

$$\mathcal{J}_H(\rho) = e^{\frac{\beta}{2}H}\rho\, e^{\frac{\beta}{2}H} \ , \tag{3.19}$$

*with an inverse given by*

$$\mathcal{J}_H^{-1}(\rho) = e^{-\frac{\beta}{2}H}\rho\, e^{-\frac{\beta}{2}H} \ . \tag{3.20}$$

In relation to the map defined in Eq. (3.18), we define the associated *backwards* quantum map as:

$$\Theta_{SW}(\rho_{SW}) = \mathrm{tr}_B\left[U^\dagger\left(\rho_{SW}\otimes\frac{e^{-\beta H_B}}{Z_B}\right)U\right] . \tag{3.21}$$

Now we introduce the standard concept of the *dual* of a quantum map:

**Definition 15** (Dual map)**.** *Any quantum map can be written in a non-unique Kraus form*

$$\Theta(\rho) = \sum_k A_k\rho A_k^\dagger \tag{3.22}$$

*with the constraint on the Kraus operators $A_k$*

$$\sum_k A_k^\dagger A_k = \mathbb{I} \tag{3.23}$$

*The dual of a map is thus defined as*

$$\Theta^*(\rho) = \sum_k A_k^\dagger\rho A_k \ . \tag{3.24}$$

*We note that this definition is independent of the particular Kraus decomposition.*

Given this dual map, we are able to prove our first quantum analogue of Crooks theorem, one of the central results of the chapter.

**Theorem 14** (Quantum Crooks)**.** *The forward and backward maps, respectively $\Gamma_{SW}$ and $\Theta_{SW}$, are related via*

$$\mathcal{J}_{H_S'+H_W}\Gamma_{SW}\mathcal{J}^{-1}_{H_S+H_W} = \Theta^*_{SW} \ . \tag{3.25}$$

*Proof.* Let us define the energy eigenbasis of the bath as $|b\rangle$ such that $\tau_B = \sum_b |b\rangle\langle b|\frac{e^{-\beta E_b}}{Z_B}$. We may write the reversed map as

$$\Theta_{SW}(\rho_{SW}) = \mathrm{tr}_B\left[U^\dagger\left(\rho_{SW}\otimes\frac{e^{-\beta H_B}}{Z_B}\right)U\right] \tag{3.26}$$

$$= \sum_{b,b'}\frac{e^{-\beta E_b/2}}{\sqrt{Z_B}}\langle b'|U^\dagger|b\rangle(\rho_{SW})\langle b|U|b'\rangle\frac{e^{-\beta E_b/2}}{\sqrt{Z_B}}, \tag{3.27}$$

from which we see that the Kraus operators are given by $\frac{e^{-\beta E_b/2}}{\sqrt{Z_B}}\langle b'|U^\dagger|b\rangle$. Therefore the dual is

$$\Theta^*_{SW}(\rho_{SW}) = \sum_{b,b'}\langle b|U|b'\rangle\frac{e^{-\beta E_b/2}}{\sqrt{Z_B}}\rho_{SW}\frac{e^{-\beta E_b/2}}{\sqrt{Z_B}}\langle b'|U^\dagger|b\rangle \tag{3.28}$$

$$= \mathrm{tr}_B\left[\frac{e^{-\beta\frac{H_B}{2}}}{\sqrt{Z_B}}U\left(\rho_{SW}\otimes\mathbb{I}_B\right)U^\dagger\frac{e^{-\beta\frac{H_B}{2}}}{\sqrt{Z_B}}\right]. \tag{3.29}$$

Hence we write

$$\mathcal{J}_{H'_S+H_W}\Gamma_{SW}\mathcal{J}^{-1}_{H_S+H_W} \tag{3.30}$$

$$= \mathrm{tr}_B\left[e^{\frac{\beta}{2}(H'_S+H_W)}U\left(e^{\frac{-\beta}{2}(H_S+H_W)}\rho_{SW}e^{\frac{-\beta}{2}(H_S+H_W)}\otimes\frac{e^{-\beta H_B}}{Z_B}\right)U^\dagger e^{\frac{\beta}{2}(H'_S+H_W)}\right] \tag{3.31}$$

$$= \mathrm{tr}_B\left[\frac{e^{-\beta\frac{H_B}{2}}}{\sqrt{Z_B}}U\left(\rho_{SW}\otimes\mathbb{I}_B\right)U^\dagger\frac{e^{-\beta\frac{H_B}{2}}}{\sqrt{Z_B}}\right] \tag{3.32}$$

$$= \Theta^*_{SW}\ , \tag{3.33}$$

where in the first line we have used the definition of $\Gamma_{SW}$, and in going from the second to the third line we used the property of conservation of energy. □

This shows that the dual map is analogous to the *transpose* or *recovery map* that appears in various results of quantum information theory [142, 17], in the context of the question of recovering quantum information after some irreversible quantum map has been applied. We postpone the exact definition of this transpose map to Chapter 4, where it will also be relevant.

Starting from Theorem 14 we can show a variety of quantum identities that, as we will see, can be thought of as the quantum analogues of quasiclassical fluctuation relations. Their names and significance will become clearer after we specialize to their form for quasiclassical states.

In particular we have:

**Theorem 15** (Quantum identities)**.** *The following quantum identites are true for thermal operations that are translation invariant on the battery.*

- *(Quantum Gibbs-stochasticity) If* $\Gamma_{SW}$ *is a thermal operation, then*

$$\mathrm{Tr}_W\left[\left(\mathcal{J}_{H'_S+H_W}\Gamma_{SW}\mathcal{J}^{-1}_{H_S+H_W}\right)(\mathbb{I}_S\otimes\rho_W)\right]=\mathbb{I}_S \tag{3.34}$$

  *for any initial state of the battery* $\rho_W$*.*

- *(Quantum entropy production equality) If* $\Gamma_{SW}$ *is a thermal operation, then, for every pair of initial states* $\rho_S,\rho_W$*, we have*

$$\mathrm{Tr}_{SW}\Big[\Big(\mathcal{J}_{T\ln\rho'_S}\mathcal{J}_{H'_S+H_W}\Gamma_{SW}\mathcal{J}^{-1}_{H_S+H_W}\mathcal{J}^{-1}_{T\ln\rho_S}\Big)(\rho_S\otimes\rho_W)\Big]=1 \tag{3.35}$$

  *where*

$$\rho'_S=\mathrm{Tr}_W[\Gamma_{SW}(\rho_S\otimes\rho_W)] \tag{3.36}$$

  *is the final state of the system.*

- *(Quantum Jarzynski equality) If* $\Gamma_{SW}$ *is a thermal operation then*

$$\mathrm{tr}_{SW}\left[\left(\mathcal{J}_{H_W}\Gamma_{SW}\mathcal{J}^{-1}_{H_S+H_W}\mathcal{J}^{-1}_{T\ln\rho_S}\right)(\rho_S\otimes\rho_W)\right]=Z'_S \tag{3.37}$$

  *for every pair of initial states* $\rho_S,\rho_W$*.*

*Proof.* Using Theorem 14 we have that

$$\mathrm{Tr}_W\left(\mathcal{J}_{H'_S+H_W}\Gamma_{SW}\mathcal{J}^{-1}_{H_S+H_W}\right)(\mathbb{I}_{SW})=\mathrm{Tr}_W\Theta^*_{SW}(\mathbb{I}_{SW})\ =\mathbb{I}_S. \tag{3.38}$$

Considering that the thermal operation (and therefore its dual as well) have the property of translation invariance, we may substitute $\mathbb{I}_{SW}$ in Eq. (3.38) with a more general state on the battery $\mathbb{I}_S\otimes\rho_W$, thus arriving to Eq. (3.34).

Next, we use the identities $\mathcal{J}^{-1}_{T\ln\rho}(\rho)=\mathbb{I}$ and $\mathrm{tr}_S\left[\mathcal{J}_{T\ln\rho}(\mathbb{I})\right]=1$, which hold for any full-rank state $\rho$. In the case where the initial state $\rho_S$ is not full rank, we can take a full rank state which is $\epsilon$ close to it, and then take the limit $\epsilon\to 0$.

From Eq. (3.38), applying $\mathcal{J}_{T\ln\rho'_S}$ and taking the trace over $S$ on both sides we obtain:

$$\mathrm{Tr}_{SW}\Big[\Big(\mathcal{J}_{T\ln\rho'_S}\mathcal{J}_{H'_S+H_W}\Gamma_{SW}\mathcal{J}^{-1}_{H_S+H_W}\mathcal{J}^{-1}_{T\ln\rho_S}\Big)(\rho_S\otimes\rho_W)\Big]=1. \tag{3.39}$$

Note that the choice of $\rho'_S$ in the expression above is arbitrary: the identity holds for any other quantum state. We however, choose this one as it will give the right physical significance to the identity.

Similarly, to derive the Jarzynski equality from Eq. (3.38) we use the identity $\mathcal{J}_{T\ln\rho}^{-1}(\rho) = \mathbb{I}$ and apply $\mathcal{J}_{H_S'}^{-1}$ outside. Then, taking the trace over $S$ on both sides we obtain:

$$\mathrm{tr}_{SW}\left[\left(\mathcal{J}_{H_W}\Gamma_{SW}\mathcal{J}_{H_S+H_W}^{-1}\mathcal{J}_{T\ln\rho_S}^{-1}\right)(\rho_S\otimes\rho_W)\right] = Z_S' \tag{3.40}$$

□

## 3.4 Quasi-classical identities

We will now go from the fully quantum identities to ones which are applicable for quasi-classical states. We thus consider the case where there is an eigenbasis $|E_i\rangle$ for $H_S$ and an eigenbasis $|E_j'\rangle$ for $H_S'$ such that

$$\Gamma_{SW}(|E_i\rangle\langle E_i|\otimes|0\rangle\langle 0|) = \sum_{j,w} P(j,w)|E_j'\rangle\langle E_j'|\otimes|w\rangle\langle w|\ , \tag{3.41}$$

where $|w\rangle$ are eigenstates of $H_W$. The fact that $\Gamma_{SW}$ maps energy eigenstates to mixtures of energy eigenstates follows from Theorem 1.

Again note that when $H_S$ or $H_S'$ are degenerate, they could have other eigenbases not satisfying the above. However, because we can rotate those coherences out as in Eq. (1.26), we shall not pay special attention to these particular cases.

We then say that $\Gamma_{SW}$ is a process which acts on quasi-classical states. Also, the independence of the position of the battery allows us to choose its initial state to be $|0\rangle$ without loss of generality.

Given that Eq. (3.41) holds, we can represent the action of the thermal operation $\Gamma_{SW}$ on quasiclassical states by the following stochastic matrix

$$P(j,w|i) = \mathrm{Tr}\left[|E_j'\rangle\langle E_j'|\otimes|w\rangle\langle w|\,\Gamma_{SW}(|E_i\rangle\langle E_i|\otimes|0\rangle\langle 0|)\right]\ . \tag{3.42}$$

Given that $\Gamma_{SW}$ is CPTP, we have that this matrix has positive entries, and also that

$$\sum_{j,w} P(j,w|i) = 1. \tag{3.43}$$

We now arrive to the central result of this section:

**Theorem 16** (Generalised Gibbs-stochasticity)**.** *The stochastic matrix $P(j,w|i)$ represents a thermal operation mapping quasi-classical states to quasi-classical states if and only if*

$$\sum_{i,w} P(j,w|i)\, \mathrm{e}^{\beta(E'_j - E_i + w)} = 1 \tag{3.44}$$

*for all $j$.*

*Proof.* The proof of the *only if* direction follows from Theorem 14 and the definition of Eq. (3.42).

$$\begin{aligned}
P(j,w|i) &= \mathrm{Tr}\left[|E'_j\rangle\langle E'_j| \otimes |w\rangle\langle w|\, \Gamma_{SW}(|E_i\rangle\langle E_i| \otimes |0\rangle\langle 0|)\right] && (3.45)\\
&= \mathrm{Tr}[|E'_j\rangle\langle E'_j| \otimes |w\rangle\langle w| \mathcal{J}^{-1}_{H'_S+H_W} \Theta^*_{SW} \mathcal{J}_{H_S+H_W}(|E_i\rangle\langle E_i| \otimes |0\rangle\langle 0|)] && (3.46)\\
&= e^{\beta(E_i - E'_j - w)} \mathrm{Tr}[|E'_j\rangle\langle E'_j| \otimes |w\rangle\langle w| \Theta^*_{SW}(|E_i\rangle\langle E_i| \otimes |0\rangle\langle 0|)], && (3.47)\\
&= e^{\beta(E_i - E'_j - w)} \mathrm{Tr}[|E'_j\rangle\langle E'_j| \otimes |0\rangle\langle 0| \Theta^*_{SW}(|E_i\rangle\langle E_i| \otimes |-w\rangle\langle -w|)], && (3.48)
\end{aligned}$$

where in the last line we have used the translation invariance property of the map. Due to the fact that $\Theta_{SW}$ is a quantum map, its dual $\Theta^*_{SW}$ is a unital map, and hence

$$\sum_{i,w} \mathrm{Tr}[|E'_j\rangle\langle E'_j| \otimes |0\rangle\langle 0| \Theta^*_{SW}(|E_i\rangle\langle E_i| \otimes |-w\rangle\langle -w|)] = 1. \tag{3.49}$$

Substituting Eq. (3.45) there, we obtain Eq. (3.44).

The *if* direction is proven assuming we have access to an infinite bath as described in Section 1.4. Let us consider a bath with infinite volume in a thermal state at inverse temperature $\beta$. As show in Sections 1.1.1 and 1.4, this and the fact that its heat capacity is infinite (due to the infinite volume) implies that the density of states $\Omega(E)$ is proportional to $e^{\beta E}$.

Due to energy conservation and invariance of the position of the battery, the joint map of system, bath and battery can be characterised by a map on joint system and bath states microstates $\pi : (i,b) \to (j,b')$ where $(i,b)$ and $(j,b')$ label pairs on system and bath energy levels, with energy $E_i + E_b$ and $E'_j + E_{b'}$ respectively.

For a given stochastic matrix $P(j,w|i)$, we can construct the map $\pi$ in the following way. When the system makes the transition $i \to j$, a fraction $P(j, w = E_b - E_{b'} + E_i - E'_j|i)$ of the bath states with energy $E_b$ are mapped to bath states with energy $E_{b'}$, for all values of $E_b$.

Using the fact that the number of states with energy $E_b$ is $\Omega(E_b) = A\, e^{\beta E_b}$ (for some constant $A$), we will now show that $\pi$ is a permutation.

The number of (final) states in the set $\{(j, b') : E_{b'} = E'\}$ is $\Omega(E_{b'})$. And the number of (initial) states $(i, b)$ that are mapped to this set is

$$\begin{aligned} & \sum_{i,E_b} P(j, w = E_b - E_{b'} + E_i - E'_j|i)\, \Omega(E_b) \\ = & \sum_{i,w} P(j, w|i)\, A\, e^{\beta(E'_j - E_i + w + E_{b'})} \\ = & \; A e^{\beta E_{b'}} = \Omega(E_{b'}) \;, \end{aligned}$$

where from the first to the second line we just change the variable over which we sum, and in the last line we use Eq. (3.44). This way we obtain exactly the number of microstates of the bath with energy $E_{b'}$. Therefore, given the stochastic matrix, and the infinite bath guaranteeing all the microstates we need, we can always find a permutation of microstates that does the transformation we want. This completes the proof. □

Note that Theorem 16 gives a necessary and sufficient condition that thermal operations with a fluctuating battery must satisfy for transformations between quasi-classical states.

**Observation 2.** *A transition from a quasiclassical state with populations $p_i$ to another $q_j$ can be done via a thermal operation that extracts a work distribution $p(w)$ if an only if there exists a matrix $P(j, w|i)$ such that*

- *It is a stochastic matrix, namely $P(j, w|i) \geq 0\, \forall j, i, w$ and*

$$\sum_{j,w} P(j, w|i) = 1. \tag{3.50}$$

- *It is a valid transformation, so it obeys the condition of Eq.* (3.44)*.*
- *It does the required transformation*

$$\sum_{w,i} P(j, w|i) p_i = q_j. \tag{3.51}$$

- *It extracts the right work distribution*

$$\sum_{i,j} P(j, w|i) p_i = p(w). \tag{3.52}$$

We shall note as a comment that the existence of this kind of matrix can be shown for particular cases via a standard technique called *linear programming.* We refer to [146] for a more thorough description of such linear programs in the context of thermal operations, and to [27] for a general reference on the topic.

When fluctuating work is involved, and provided we do not restrict the work fluctuations in any way [150], it is easy to see that any particular transition between states can be done given enough work. To see this, let us choose a particular kind of work extraction process named *thermodynamically reversible* [162, 150], in which

$$P(j,w|i) = \delta\left(w + E_i - E'_j + \frac{1}{\beta}\log\frac{p_i}{q_j}\right) P(j|i), \tag{3.53}$$

for some $P(j|i)$ such that it obeys $\sum_i P(j|i)p_i = q_j$. Using this definition in the LHS of Eq. (3.44) we can see that the constraints are obeyed by definition.

Eq. (3.44) can be seen as an extension of the Gibbs preservation condition that can be found in Theorem 1 to the case where thermodynamical work is included. In fact, when the Hamiltonian of the system does not change, and setting $w = 0$, we recover the condition of Gibbs preservation of that theorem.

In a similar fashion to the previous section, we can write the quasi-classical version of Eq. (3.37).

**Corollary 3.** *[Quasiclassical entropy production equality] A process on quasi-classical states that acts unitarily on the total system, conserves energy and is independent of the position of the battery satisfies*

$$\left\langle \mathrm{e}^{\beta(f'_j - f_i + w)} \right\rangle = 1 \ , \tag{3.54}$$

*where we define the following random variables as*

$$\begin{aligned} f_i &= E_i + \frac{1}{\beta}\ln p_i \ , && (3.55) \\ f'_j &= E'_j + \frac{1}{\beta}\ln q_j \ . && (3.56) \end{aligned}$$

*Proof.* This follows from very simple algebra. Starting from Eq. (3.44),

$$\sum_{i,w} P(j,w|i) e^{\beta(E'_j - E_i + w)} \frac{p_i q_j}{p_i q_j} = 1 \tag{3.57}$$

$$\sum_{i,w} P(j,w,i) e^{\beta(E'_j - E_i + w) - \log p_i + \log q_j} = q_j, \tag{3.58}$$

and summing over the $j$ index we obtain

$$\sum_{j,i,w} P(j,w|i)\, \mathrm{e}^{\beta(f'_j - f_i + w)} p_i = 1. \tag{3.59}$$

$\square$

Now we can invoke a simple but useful mathematical identity, named *Jensen's inequality* [97].

**Lemma 8** (Jensen's inequality)**.** *Let $f(x)$ be a convex function, $x_l$ a set of numbers in its domain, and $a_l$ a set of positive weights. The following inequality holds*

$$f\left(\frac{\sum_l a_l x_l}{\sum_l a_l}\right) \geq \frac{\sum_l a_l f(x_l)}{\sum_l a_l}. \tag{3.60}$$

*Equality holds if and only if $x_l = x\ \forall l$ or if $f$ is linear.*

Due to the convexity of the exponential, we can apply this theorem to Eq. (3.54). For this, we identify $f(x) = e^{\beta x}$, the $x_l$ are $f'_j - f_i + w$ and the weights $a_l$ are the probabilities $P(j,i,w) \equiv P(j,w|i)p_i$. We hence derive the following inequality

$$\langle f'_j - f_i + w \rangle = F(\rho) - F(\sigma) + \langle w \rangle \leq 0\ , \tag{3.61}$$

where $F(\rho) = \langle E \rangle - \frac{1}{\beta} S(\rho)$ is the free energy of the quasiclassical state $\rho$. We note that the thermodynamically reversible processes of Eq. (3.53) saturate this inequality even at the level of individual $i, j$, without doing the average.

This equation can be thought of as a version of the standard 2nd law, in so far as it gives a limit to the amount of work that can be extracted along a process.

In any case, Eq. (3.54) is significantly stronger than this inequality. For instance, it implies the following infinite list of inequalities

$$\sum_{k=1}^{N} \frac{\beta^k}{k!} \left\langle \left(f'_j - f_i + w\right)^k \right\rangle \leq 0\ , \tag{3.62}$$

where $N$ can be any odd number. Note that Eq. (3.61) is the $N = 1$ case. One can think of Eq. (3.62) as providing higher order corrections to the standard second law inequality. All the other inequalities have information about the joint fluctuations of $f_i, f'_j$ and $w$. We shall not give a full proof of Eq. (3.62) here, but we note that it follows from considering the residue of the Taylor expansion of the exponential function to any odd order, which is always positive.

From the second statement of Jensen's inequality (the "only if" statement), it can be shown that the saturation of the 2nd law

$$\left\langle f'_j - f_i + w \right\rangle = 0 \ , \tag{3.63}$$

implies

$$w = f_i - f'_j \ \text{ for all } i, j, \tag{3.64}$$

and hence the *thermodynamically reversible* processes not only saturate the 2nd law inequality, but are the only ones doing so. Thus, they provide the optimal consumption or extraction of work when we take its average $\langle w \rangle$ as the figure of merit.

Outside of the thermodynamically reversible regime, violations of

$$f'_j - f_i + w \leq 0 \ , \tag{3.65}$$

for individual realizations of the process $(i, j, w)$ can occur. Defining the *excess* random variable $v = f'_j - f_i + w$ (which can be identified as the negative of the *entropy production* [159]), allows us to write Eq. (3.54) as

$$\left\langle \mathrm{e}^{\beta v} \right\rangle = 1 \ . \tag{3.66}$$

Recalling that the exponential function gives more weight to the positive fluctuations as compared with the negative ones, we conclude that, outside of the thermodynamically reversible regime, the negative fluctuations of $v$ must be larger and/or more frequent than the positive ones. In other words: *the violation of the second law is exponentially more rare than its satisfaction.* This asymmetry is also articulated by the infinite list of bounds for the moments of $v$ given in Eq. (3.62).

Next we proceed to obtain the classical version of Result 15.

**Corollary 4** (Quasiclassical Jarzynski Equality)**.** *A process on quasi-classical states that acts unitarily on the total system, conserves energy and is independent of the position of the battery satisfies*

$$\left\langle \mathrm{e}^{\beta(w - f_i)} \right\rangle = Z'_S \ . \tag{3.67}$$

*Proof.* Starting from Eq. (3.44) the derivation just involves very simple algebra. Multiply and divide within the sum by $p_i$ to get $\log p_i$ in the exponent, multiply on both sides by $e^{-\beta E'_j}$ and then sum over the $j$ index. The result is

$$\sum_{i,j,w} P(j,w|i) p_i e^{\beta(w-f_i)} = Z'_S. \tag{3.68}$$

$\square$

Note that this version of the Jarzynski equation is valid for any initial state of the system, encoded in the fine-grained free energy $f_s$. For the particular case where the initial state is thermal, we have $\mathrm{e}^{-\beta f_i} = Z_S \;\; \forall i$, which implies the standard Jarzynski equality

$$\left\langle \mathrm{e}^{\beta w} \right\rangle = \frac{Z'_S}{Z_S} \; . \tag{3.69}$$

This is the standard statement of the Jarzynski equality, which coincides in form with the one derived in Corollary 1. We note however a big difference between the two cases: in the previous version the work random variable was defined via projective energy measurements in system and bath, whereas here the work is defined more explicitly, as an energy change in the battery.

### 3.4.1 Quasiclassical Crooks theorem

We can now recover a quasiclassical Crooks relation from the quantum version in Theorem 14.

First, let us define the stochastic matrix associated with the reversed process as

$$P_{\text{back}}(i,-w|j) = \mathrm{Tr}[\Theta_{SW}(|E'_j\rangle\langle E'_j| \otimes |w\rangle\langle w|)|E_i\rangle\langle E_i| \otimes |0\rangle\langle 0|], \tag{3.70}$$

which is a natural definition given that for the forward process in Eq. (3.42).

The relation is a prelude to Crooks' theorem, and is contained in the following theorem.

**Theorem 17.** *The stochastic matrices associated to forward and backwards thermal operations with fluctuating work are related as*

$$P_{\text{back}}(i,-w|j) = P(j,w|i)\, \mathrm{e}^{\beta(E'_j - E_i + w)} \; . \tag{3.71}$$

*Proof.* Starting from Eq. (3.25), we apply the identity to a state $|E_i\rangle\langle E_i| \otimes |0\rangle\langle 0|$, multiply outside by $|E'_j\rangle\langle E'_j| \otimes |w\rangle\langle w|$ and take the trace. We then obtain

$$\begin{aligned} &\mathrm{Tr}[|E'_j\rangle\langle E'_j| \otimes |w\rangle\langle w| \mathcal{J}_{H'_S+H_W} \Gamma_{SW} \mathcal{J}^{-1}_{H_S+H_W}(|E_i\rangle\langle E_i| \otimes |0\rangle\langle 0|)] \\ &= \mathrm{Tr}[|E'_j\rangle\langle E'_j| \otimes |w\rangle\langle w| \Theta^*_{SW} \; (|E_i\rangle\langle E_i| \otimes |0\rangle\langle 0|)]. \end{aligned} \tag{3.72}$$

The projectors commute with the operators $J^{-1}_{H_S+H_W}$ and $J_{H'_S+H_W}$, and their total effect is that of picking up a factor $e^{\beta(E'_j-E_i+w)}$. Then, applying the definition of the stochastic matrices given in Eq. (3.42), and using the definition of the backwards stochastic matrix of Eq. (3.70), we arrive at Eq. (3.71). □

One can check that the constraint in Eq. (3.44) applied to $P\left(j,w|i\right)$ is equivalent to the normalization of $P_{\text{back}}\left(i,-w|j\right)$, and the normalization of $P\left(j,w|i\right)$ is equivalent to the constraint in Eq. (3.44) applied to $P_{\text{back}}(i,-w|j)$. This by itself implies that $P_{\text{back}}(i,w|j)$ is a thermal operation, and hence, there is a global unitary generating this transformation. As we have seen, one can use the unitary that is the inverse of the one that generates $P(j,w|i)$. However, other unitaries may also generate the same dynamics on system and battery, and may hence also qualify as relevant backwards processes. For examples of what these may look like we refer the reader to [3].

By defining the probability of obtaining work $w$ in going from energy level $E_i$ to $E'_j$ when the initial state is thermal by $p_{\text{forward}}(w,j,i)=P(j,w|i)e^{-\beta E_i}/Z_S$ for the forward process and $p_{\text{back}}(-w,j,i)=P_{\text{back}}(i,-w|j)e^{-\beta E'_j}/Z'_S$ for the reverse, we obtain a Crooks relation

$$\frac{p_{\text{forward}}(w,i,j)}{p_{\text{back}}(-w,j,i)}=e^{-\beta w}\frac{Z'_S}{Z_S} \tag{3.73}$$

without needing to assume micro-reversibility, which is the starting assumption of [46, 47]. One can take $p_{\text{back}}(-w,i,j)$ to the RHS of Eq. (3.73) and then sum over $i$ and $j$ to obtain the more standard Crooks relation

$$\frac{p_{\text{forward}}(w)}{p_{\text{back}}(-w)}=e^{-\beta w}\frac{Z'_S}{Z_S} \tag{3.74}$$

but Eq. (3.73) is slightly more general. Again, Eq. (3.74) has the same form as the Tasaki-Crooks equation in Theorem 12, but here the work random variable is associated to a change of energy in the battery along a particular run of the protocol, as opposed to the difference in the result of two projective energy measurements.

### 3.4.2 Connection with fluctuations of states

The upper bound of Theorem 11 can be related to the Jarzynski equality, when the thermal operations are applied to the system in an initial thermal state. For simplicity let us focus on the case where the Hamiltonian does not change (otherwise a correction of $\log \frac{Z'_S}{Z_S}$ must be added to the work). The equality reads

$$\langle e^{\beta w} \rangle = \sum_w e^{\beta w} p(w) = 1. \tag{3.75}$$

Again this is valid if the initial state is thermal, so let us take the special case of Theorem 11, of a process where we start with a thermal state $\tau$ and probabilistically go to some quasiclassical $\sigma$, with optimal probability $p^*$. Because $\tau$ is the steady state, the effect of that operation is trivial:

$$\tau \xrightarrow{TO} \rho' = \tau = p^* \sigma + (1 - p^*) X. \tag{3.76}$$

Now, if we append a battery with Hamiltonian $H_W = \int_{\mathbb{R}} dw\, w |w\rangle\langle w|$ as a work storage system initially in the state $|0\rangle$, by definition there exists a different set of thermal operations that extracts work $W_{\sigma \to \tau}$ from $\sigma$

$$\sigma \otimes |0\rangle\langle 0| \xrightarrow{TO} \tau \otimes |W_{\sigma\to\tau}\rangle\langle W_{\sigma\to\tau}|. \tag{3.77}$$

By linearity, applying this set of TO to $\tau = p^*\sigma + (1 - p^*)X$ yields:

$$p^* \tau \otimes |W_{\sigma\to\tau}\rangle\langle W_{\sigma\to\tau}| + (1 - p^*) X'_{sw}, \tag{3.78}$$

where $X'_{SW}$ is some joint system-battery state, with the battery in some work distribution $p_X(w)$. Note that this operation is applied on both system and battery, and does not need to conserve the thermal state of the system alone. The Jarzynski equality for this operation reads:

$$p^* e^{\beta W_{\sigma\to\tau}} + (1 - p^*) \sum_w p_X(w) e^{\beta w} = 1. \tag{3.79}$$

The second term in this sum is positive, and hence we have:

$$p^* e^{\beta W_{\sigma\to\tau}} \leq 1, \tag{3.80}$$

which is the upper bound of Theorem 11.

Note that in situations where the upper bound is saturated (such as reversible processes with $W_{\sigma\to\tau} = -W_{\tau\to\sigma}$, when the thermomajorization curve of $\sigma$ is also a straight line) the operation in Eq. (3.77) costs a negative and divergent amount of work in the case of failure i.e. from the state $X$ in Eq. (3.76) (as the positive sum $\sum_w p_X(w) e^{\beta w}$ is forced to be zero). This kind of particular case is the focus of the next section.

## 3.5 Deterministic work: Landauer erasure revisited

The generalised Gibbs-stochastic condition of Eq. (3.44) gives more information than the Jarzynski equation or the entropy production fluctuation theorem, as the number of constraints it imposes is given by the dimension of the system.

As a concrete and simple example of these conditions, let us take the case of Landauer erasure [107]. We consider a qubit with trivial Hamiltonian $H_S = 0$ that is initially in the maximally mixed state and which we want to map to the $|0\rangle$ state. Recalling that a positive work value represents a yield, while a negative work value is a cost, we consider a process such that $-w_0$ is the work cost when erasing $|0\rangle \to |0\rangle$, and $-w_1$ the work cost if the transition $|1\rangle \to |0\rangle$ occurs. We allow for an imperfect process and imagine that this erasure process happens with probability $1-\epsilon$, while with probability $\epsilon$ we have an error and either $|0\rangle \to |1\rangle$ with work yield $\bar{w}_0$ or $|1\rangle \to |1\rangle$ with work yield $\bar{w}_1$. We call such a process *deterministic*, because the value of $w$ is completely determined by the particular transition of the system's state. For this scenario, the generalised Gibbs-stochastic condition, Eq. (3.44), gives two conditions

$$e^{\beta w_o} + e^{\beta w_1} = 1/(1-\epsilon) \tag{3.81}$$

$$e^{\beta \bar{w}_o} + e^{\beta \bar{w}_1} = 1/\epsilon. \tag{3.82}$$

We immediately see that to obtain perfect erasure, $\epsilon \to 0$, then when the erasure fails there must be work fluctuations which scale like $-T \log \epsilon$. Such a work gain happens rarely, but precludes perfect erasure, and is related to the third law of thermodynamics as proven in [124] and discussed in detail in [150].

In the limit of perfect erasure, we easily see that the minimal average work cost of erasure, $T \log 2$, is obtained when the work fluctuations associated with successful erasure are minimal (that is, when $w_0 = w_1 = T \log 2$). We also see that no work, not even probabilistically, can be obtained in such a deterministic process.

Through this example, one sees that the identities proven here can lead to new insights in thermodynamics, particularly with respect to work fluctuations and their quantum aspects.

## 3.6 Outlook

We have shown a way to define work within the resource-theoretic setting such that fluctuation theorems appear when looking at quasiclassical states. This allowed us to infer the quantum shape of fluctuation theorem in this context, as expressions that reduce to the classical ones when all the states involved are quasiclassical. However, beyond that limit we do not have a very precise understanding of the meaning of identities such as those found in Theorem 15. For instance, it is not clear whether a useful quantum analogue of Jensen's inequality exists that allows us to derive inequalities between quantum operators reminiscent of the second law the way we obtained Eq. (3.61). For instance, a Jensen's operator inequality found in [82] does not seem to be enough, and further tools are needed.

The definition of work given here involves a battery with an associated translation operator. To formally define such an operation, an infinite-dimensional battery, with a ground state potentially unbounded from below, is needed. This is of course an idealization, and it remains to be seen which kind of systems approximate such a construction well. This problem seems to be very directly related to that of finite-sized clocks in quantum mechanics [194], where a perfect clock can only be a system with a Hamiltonian that is unbounded from below.

There are kinds of fluctuation theorems that we have not mentioned in this chapter, such as those involving non-equilibrium steady states [161], and exchange fluctuation theorems [95]. As a further avenue of research within this resource-theoretic approach, one would like to know how may these different kinds fit within the framework. Even beyond fluctuation theorems, issues such as multiple baths and non-equilibrium steady states are yet to be put under the light of the resource-theoretic perspective.

## 3.7 Summary

In this chapter we have motivated and introduced the very important topic of work fluctuations, and showed how it can be incorporated into the resource theory. The aim of this is to bridge the resource theoretic approach to nonequilibrium thermodynamics with more traditional approaches, via incorporating versions of some of their most renowned results: the fluctuation theorems.

In order to do this, we have defined the key property of translational invariance, and showed how from it a number of fluctuation theorems follow, in particular when one looks at quasiclassical states. We also give the quantum expressions from which the quasiclassical ones follow.

The primitive of all these results is the statement of the quantum Crooks theorem (Theorem 14). This is a relation between a forward and a backward operation, which turns out to be connected to the notion of transpose (or recovery) map from quantum information theory.

We also show some consequences that these work fluctuations have for the previous notion of deterministic work, and in particular for Landauer erasure. We see that when we consider work fluctuations, a protocol in which deterministic work is extracted has a very large work fluctuation, that happpens with a very low probability. This statement can be seen as a version of the third law of thermodynamics.

# Chapter 4

# Convergence to equilibrium and recovery of quantum information

We now proceed with a slightly different topic, which can nevertheless be embedded in the resource-theoretic formulation of thermodynamics. We will now be specializing in a particular case of dynamical evolutions called Davies maps, which describe the dynamics of a system weakly coupled to a heat bath. These maps are used thoroughly in the open quantum systems literature [34, 151], and frequently appear as models of thermal noise in quantum informational settings [10, 11, 44]. Throughout this chapter, we will not limit ourselves to quasiclassical states, but to general quantum states and evolutions.

First, we shall introduce two concepts: the idea of a recovery map in quantum information, and the entropy production when a system is coupled to a heat bath.

## 4.1 Recovery of quantum information

In Section 3.3 of Chapter 3 we said that the form of the result of Theorem 14 connects the statement of quantum fluctuation theorems with a notion that appeared in quantum information named a *recovery map*. In this section we shall delve into this notion by explaining some results in quantum information that introduce and motivate it, after which its use in the context of non-equilibrium physics will become clearer.

The key quantity of this section is the quantum relative entropy, which is defined as

$D(\rho||\sigma) = \mathrm{Tr}[\rho\big(\log\rho - \log\sigma\big)]$. It obeys the key property of the *data processing inequality*, also referred to as contractivity

**Theorem 18** (Data processing inequality)**.** *Let $T(\cdot)$ be a quantum map. The quantum relative entropy does not increase,*

$$D(\rho||\sigma) \geq D(T(\rho)||T(\sigma)). \tag{4.1}$$

This is an important property that states that two states become harder to distinguish after applying a quantum map, which is generally irreversible. The reason for this is that the relative entropy measures with what probability can $\rho$ be mistaken by $\sigma$ in a hypothesis testing setting (the exact statement is the quantum analogue of Sanov's theorem, and can be found in [86]).

Now let us introduce a seminal theorem by Petz, shown in [142], and first written in the present form in [84].

**Theorem 19** (Petz's theorem)**.** *Let $\rho, \sigma$ be quantum states, and $T(\cdot)$ a quantum map. The relative entropy does not decrease, namely*

$$D(\rho||\sigma) = D(T(\rho)||T(\sigma)). \tag{4.2}$$

*if and only if there exists a quantum map $\tilde{T}$ such that both states are recovered: $\tilde{T}(T(\rho)) = \rho$ and $\tilde{T}(T(\sigma)) = \sigma$. Moreover, $\tilde{T}$ can always be taken to be the map*

$$\tilde{T}(\cdot) = \sigma^{1/2}T^{*}\left(T(\sigma)^{-1/2}\cdot T(\sigma)^{-1/2}\right)\sigma^{1/2}. \tag{4.3}$$

Essentially this theorem tells us that when the relative entropy does not decrease after a quantum evolution, that quantum evolution can be undone on the particular pair of states $\rho$ and $\sigma$. That is, we are able to *recover* both $\rho$ and $\sigma$. We note that $\sigma$ is recovered by the definition in Eq. (4.3) and the fact that $T^{*}(\mathbb{I}) = \mathbb{I}$, so the non-trivial part of the theorem is the fact that $\rho$ is recovered. The map $\tilde{T}$ is usually referred to as Petz's recovery map.

In recent times considerable efforts have been focused towards giving useful strengthenings of this theorem. The aim has been to show an approximate version of this theorem that reads: when the relative entropy does not decrease very much, the state $\rho$ can be recovered not perfectly, but with high precision.

Recent works that have gone in this direction are [190, 99, 170, 68]. We here will state the currently strongest instance of this theorem, shown in [169].

**Theorem 20.** *The decrease of relative entropy is lower bounded as*

$$D(\rho||\sigma) - D(T(\rho)||T(\sigma)) \geq D_{\mathbb{M}}(\rho||\tilde{T}'T(\rho)), \tag{4.4}$$

*where the map $\tilde{T}'$ is the Rotated Petz recovery map, defined as*

$$\tilde{T}'(\cdot) = \int_{-\infty}^{\infty} dt p(t) \tilde{T}'_t(\cdot) \tag{4.5}$$

*with $p(t) = \frac{\pi}{2}(\cosh(\pi t) + 1)^{-1}$ a probability distribution and*

$$\tilde{T}'_t = \sigma^{1/2+it} T^*(T(\sigma)^{-1/2-it} \cdot T(\sigma)^{-1/2+it})\sigma^{1/2-it}. \tag{4.6}$$

*The measured relative entropy $D_{\mathbb{M}}(\rho||\sigma)$ is defined as*

$$D_{\mathbb{M}}(\rho||\sigma) = \sup_M D(P_{\rho,M}||P_{\sigma,M}), \tag{4.7}$$

*where the optimization is over the whole set of POVMs $M$ with individual positive operators $M(x)$ such that $\sum_x M(x) = \mathbb{I}$, and $P_{\rho,M}(x) = \mathrm{Tr}[\rho M(x)]$ is a probability distribution. The relative entropy in the RHS of Eq.* (4.4) *is therefore a classical one.*

From this result we can recover Theorem 19 as a corollary, in the particular case in which the relative entropy does not decrease, and hence the measured relative entropy is zero, implying both inputs are identical. Therefore, this result can be seen as a simultaneous strengthening of Petz's theorem and of the data processing inequality.

It was thought for some time that this was not the strongest version of this theorem. In fact, it was conjectured in [108] that

**Conjecture 1** (Li-Winter conjecture)**.** *Let $\rho, \sigma$ be quantum states, and $T(\cdot)$ a quantum map. The following inequality holds*

$$D(\rho||\sigma) - D(T(\rho)||T(\sigma)) \geq D(\rho||\hat{T}(\rho)), \tag{4.8}$$

*for some map $\hat{T}$ such that $\hat{T}(T(\sigma)) = \sigma$.*

The analogue for classical stochastic channels of this inequality is true and straightforward to prove [108]. However, as was partially shown in [31] and with full generality in [67], it is not true for general quantum maps. In the course of this chapter, however, we will find that it is indeed true for Davies maps, adding to those in [7, 37].

The main initial motivation for proving such an inequality was the particular case of states and maps in which the decrease of relative entropy turns into the conditional mutual information, which was thought to be very useful for a big number of applications, ranging from many body physics [101] and entanglement theory [108] or quantum algorithms [32]. The first version of this result was first shown by Fawzi and Renner in [68] and is considered one of the most important results in quantum information theory in recent times.

How are these ideas useful for thermodynamics? A result of the kind of Theorem 20 tells us about how reversible an irreversible quantum evolution is in a very specific sense. The decrease of quantum relative entropy gives a measure of such irreversibility. In the context of thermodynamics, then, we will give a specific meaning to such a decrease of relative entropy and show what recoverability means in this context.

To that end, we introduce the following useful concept that appears when a system interacts with a thermal state.

## 4.2 Entropy production

We will from now on be focusing on thermodynamics situations in which only a system and a bath are involved, and, unlike the previous chapters, there is no battery or work extraction.

The important concept we now introduce is that of *entropy production*, which we define as

$$\Delta S + \beta \Delta Q, \tag{4.9}$$

where $\Delta S$ is the change of entropy in the system, and $\Delta Q$ is the change of energy of the bath (the $\Delta$ indicates the difference between final and initial).

In general, we have that, if $\Delta S_B$ is the change of entropy in the bath [26]

$$\Delta S_B \geq \beta \Delta Q, \tag{4.10}$$

with equality when the process is quasistatic. Because the bath is very large, the change induced by the system will be small compared to it, and hence we can expect the processes at hand to be close to quasistatic, and the inequality in Eq. (4.10) be close to saturated. This justifies naming the quantity of Eq. (4.9) as entropy production, as it is close to the sum of the two changes of local entropy.

If the evolution is unitary, however, the total entropy of system and bath together does not change. Because of this, the entropy production defined above can only be understood as a measure of irreversibility if we neglect some factors, such as the correlations between system and bath. This is expressed in the following result, which can be found in both [64, 144].

**Theorem 21.** *Let a system and a bath initially in a product state* $\rho_S \otimes \tau_\beta$ *evolve under some joint unitary dynamics* $U$*. The entropy production of the evolution is equal to*

$$\Delta S + \beta \Delta Q = I(S' : B') + D(\tau' || \tau_\beta), \tag{4.11}$$

*where the first term is the mutual information* $I(S' : B') = S(\sigma_S) + S(\tau') - S(U \rho_S \otimes \tau_\beta U^\dagger)$ *between system and reservoir after the unitary evolution, and the second term is the relative entropy difference between the final and initial states of the reservoir, which we label as* $\tau', \tau_\beta$*.*

*Proof.* The proof can be found in both [64, 144] and follows from some elementary manipulations.

Let $\rho_S$ and $\sigma_S$ be the initial and final states of the system, we can write

$$S(\rho_S) - S(\sigma_S) + I(S' : B') \tag{4.12}$$

$$= S_B(\tau') - S_B(\tau_\beta) \tag{4.13}$$

$$= -\mathrm{Tr}[\tau' \log \tau'] + \mathrm{Tr}\left[\tau_\beta \log \frac{e^{-\beta H_B}}{Z}\right] \tag{4.14}$$

$$= -\mathrm{Tr}[\tau' \log \tau'] - \beta \mathrm{Tr}[H_B \tau_\beta] - \log Z + \beta \mathrm{Tr}[H_B \tau'] - \beta \mathrm{Tr}[H_B \tau'] \tag{4.15}$$

$$= \beta \Delta Q - D(\tau' || \tau_\beta). \tag{4.16}$$

To go from the first line to the second we have used the definition of mutual information and the fact that the entropy is invariant under unitaries and additive under tensor product.

$$I(S' : B') = S(\sigma_S) + S(\tau') - S(U \rho_S \otimes \tau_\beta U^\dagger) \tag{4.17}$$

$$= S(\sigma_S) + S(\tau') - S(\rho_S \otimes \tau_\beta) \tag{4.18}$$

$$= S(\sigma_S) + S(\tau') - S(\rho_S) - S(\tau_\beta). \tag{4.19}$$

□

We note that each of the terms in the RHS of Eq. (4.11) encodes a different effect: the first one quantifies the correlations created between the system and the reservoir, and the second one the change of state of the bath after the joint evolution.

In the following section we will be specializing to maps in which the unitary $U$ is generated by a very weak interaction Hamiltonian. In the derivation of the Markovian evolution of Lindblad form [110, 79] of such maps various approximations are involved, but two of the more important ones are the neglection of the correlations between system and reservoir, and of the change of state of the bath.

It will be shown that here the entropy production becomes a very natural way of measuring the irreversibility of the process on the system. Given that, Theorem 21 makes the following fact explicit: the entropy produced comes from the correlations with the bath and the change of the reservoir, both of which are omitted in the effective description that the Lindbladian gives.

## 4.3 Davies maps and entropy production

We now proceed to describe the kind of Markovian maps that we will be focusing on in the rest of the chapter.

Davies maps are a particular set of quantum dynamical semigroups that describe the evolution of a system that is weakly interacting with a heat bath. The first rigorous derivation of their form was given in [53] (see [12, 151] for more modern treatments). As they are time-continuous quantum semigroups, their generator takes the form of a Lindbladian operator, which we define as

$$\frac{\mathrm{d}\rho_S(t)}{\mathrm{d}t} = \mathcal{L}(\rho_S(t)) + \mathrm{i}\theta(\rho_S(t)), \tag{4.20}$$

where $\mathcal{L}$ is called the *Lindbladian* and $\theta(\cdot) = -[H_{\text{eff}}, \cdot]$ is called the unitary part, with $H_{\text{eff}}$ the effective Hamiltonian. The Lindbladian dissipative part can be written as

$$\mathcal{L}(\rho_S(t)) = \sum_{\omega,\alpha} G^{\alpha}(\omega)\big[S^{\alpha\dagger}(\omega)\rho_S(t)S^{\alpha}(\omega) - \frac{1}{2}\{S^{\alpha\dagger}(\omega)S^{\alpha}(\omega), \rho_S(t)\}\big], \tag{4.21}$$

where the sum $\omega$ is over the energy gaps of $H_S$, and

$$e^{-itH_S}S^\alpha(\omega)e^{itH_S} = S^\alpha(\omega)e^{-i\omega t} \tag{4.22}$$

$$\tau_S S^\alpha(\omega) = e^{\beta\omega}S^\alpha(\omega)\tau_S \tag{4.23}$$

$$G^\alpha(\omega) = e^{\beta\omega}G^\alpha(-\omega). \tag{4.24}$$

The solution of Eq. (4.20) is a one-parameter family of quantum CPTP maps $M_\Delta(\cdot)$, $\Delta \geq 0$ which governs the dynamics, $M_\Delta(\rho_S(t)) = \rho_S(t+\Delta)$. The important properties that the canonical form of Davies maps, denoted $T_t(\cdot)$, possess:

1) They arise from the weak system-bath coupling limit

2) They can be written in the form $T_t(\cdot) = \mathrm{e}^{it\theta + t\mathcal{L}}(\cdot)$, with $\theta$ and $\mathcal{L}$ time independent

3) $\theta$ and $\mathcal{L}$ commute: $\theta(\mathcal{L}(\cdot)) = \mathcal{L}(\theta(\cdot))$

4) They have a thermal fixed point: $T_t(\tau_S) = \tau_S$, where $\tau_S$ is the Gibbs state of the system at temperature $\beta$.

5) Their dissipative and unitary part satisfy *Quantum detailed balance* (QDB):

$$\langle A, \mathcal{L}^*(B)\rangle_\Omega = \langle \mathcal{L}^*(A), B\rangle_\Omega, \tag{4.25}$$

$$[H_{\text{eff}}, \Omega] = 0, \tag{4.26}$$

   for all $A, B \in \mathbb{C}^{n\times n}$, where $\mathcal{L}^*$ (also sometimes written $\mathcal{L}^\dagger$) is the adjoint Lindbladian and in the case of Davies maps, $\Omega = \tau_S$. The scalar product in Eq. (4.25) is defined as

$$\langle A, B\rangle_\Omega := \mathrm{Tr}[\Omega^{1/2}A^\dagger\Omega^{1/2}B]. \tag{4.27}$$

   This is sometimes referred to as the *reversibility* or KMS condition. It is stronger than 4), since it has as a consequence that $\Omega$ is the fixed point, as $\mathcal{L}(\Omega) = 0$.

In the literature, there are various different definitions of QDB which are in general not equivalent when imposed on general maps. However, in the appendix we will show that for Davies maps the different conditions are in fact the same.

In addition to the properties above, it is sometimes assumed that:

6) The dynamics associated with Davies maps converge to the fixed point, $\lim_{t\to\infty} T_t(\rho_S(0)) = \tau_S$ for any initial state $\rho_S(0)$.

Such convergence is guaranteed if more stringent conditions are imposed on the Davies map [166, 164, 69, 70]. We however will not need to assume 6) for our results to hold.

Recall that the quantum relative entropy, in the special case that $\sigma$ is a Gibbs state, has an interpretation in terms of a free energy,

$$D(\rho(t)||\tau_S) = \beta F_\beta(\rho_S(t)) - \log Z_S, \tag{4.28}$$

where $Z_S = \mathrm{Tr}[e^{-\beta H_S}]$. We can thus write

$$D(\rho(0)||\tau_S) - D(\rho(t)||\tau_S) = \beta \left(F_\beta(\rho_S(0)) - F_\beta(\rho_S(t))\right) \tag{4.29}$$

$$= \Delta S - \beta \mathrm{Tr}[H_S(\sigma_S - \rho_S)] \tag{4.30}$$

It turns out that the quantity in Eq. (4.29) is the same as the entropy production in Eq. (4.9). Here system and bath are weakly coupled, meaning that the norm of the interaction Hamiltonian is very small. As a consequence, this evolution transfers energy between system and bath, and hence we can write $\mathrm{Tr}[H_S(\sigma_S - \rho_S)] = -\Delta Q$. Making that substitution we can see that both expressions are equal. Connecting back with Theorem 21, we can hence identify the decrease of relative entropy as the total entropy production of system and reservoir.

We now give a more detailed account of the microscopic origin of these Davies maps, and of the form of the weak coupling limit, property 1).

### 4.3.1 Microscopic origin of Davies maps

Davies maps are derived from considering the dynamics of a state $\rho_S \in \mathcal{S}(\mathcal{H}_\mathcal{S})$, where $\mathcal{H}_\mathcal{S}$ is of finite dimension $n$, in contact with a thermal bath on an infinite dimensional Hilbert space $\mathcal{H}_\mathcal{B}$.

We have to assume some technical conditions about the bath. Let $H_B$ be a Hamiltonian on $\mathcal{H}_\mathcal{B}$. Since we want thermal states associated to $H_B$ to be thermodynamically stable, we assume that $Z_B = \mathrm{Tr}[\exp(-\beta H_B)] < \infty$ for all $\beta > 0$. $H_B$ must therefore have a purely discrete spectrum, which is bounded from below and has no finite limit points; that is, there are only a finite number of energy levels in any finite interval $\Delta E$. This is consistent with our definition of the bath in Section 1.1.1, where we assumed the existence of a finite density of states $\Omega(E)$.

The quantum state $\rho_S \in \mathcal{S}(\mathcal{H_S})$ with its free self-adjoint Hamiltonian $H_S$ of finite dimension interacts with the system via a bounded interaction term $H_I$ , with a parameter $\lambda > 0$ determining the interaction strength as follows

$$H_{SB} = H_S \otimes \mathbb{I}_B + \mathbb{I}_S \otimes H_B + \lambda\, H_I. \tag{4.31}$$

The initial state on $\mathcal{S}(\mathcal{H}_S \otimes \mathcal{H}_B)$ is as usual assumed to be product, $\rho_S \otimes \tau_B$, with $\tau_B$ the Gibbs state at inverse temperature $\beta$. The Schrodinger picture dynamics of the system at time $\tilde{t}$ is given by the unitary operator

$$U(\tilde{t}) := \mathrm{e}^{-\mathrm{i}\tilde{t}H_{SB}} \tag{4.32}$$

after tracing out the environment. More precisely, by

$$\mathrm{Tr}_B \left[ U(\tilde{t})\rho_S \otimes \tau_B\, U^\dagger(\tilde{t}) \right] \in \mathcal{S}(\mathcal{H}_S), \tag{4.33}$$

where $U^\dagger$ denotes the adjoint of $U$.

The Davies map $T_t(\cdot)$ is defined by taking the limit that the interaction strength $\lambda$ goes to zero, while the time $\tilde{t}$ goes to infinity while maintaining $\tilde{t}\lambda^2 := t$ fixed. More concisely,

$$T_t(\cdot) = \lim_{\lambda \to 0^+} \mathrm{Tr}_B \left[ U(\tilde{t})(\cdot) \otimes \tau_B\, U^\dagger(\tilde{t}) \right] \in \mathcal{S}(\mathcal{H}_S) \quad \text{subject to } \tilde{t}\lambda^2 = t \text{ fixed.} \tag{4.34}$$

It is assumed that in this limit $U(\tilde{t})$ and its inverse $U^\dagger(\tilde{t})$ are still unitary operators mapping states on $\mathcal{S}(\mathcal{H}_S \otimes \mathcal{H}_B)$ to states on $\mathcal{S}(\mathcal{H}_S \otimes \mathcal{H}_B)$. To gain more physical insight into this construction, we refer to [166, 52, 53].

### 4.3.2 Davies maps are thermal operations

We now prove a Lemma that will be interesting for two reasons: we will use it in the derivation of the main result of the chapter, and it shows how the Davies maps are part of the set of thermal operations.

Essentially we show that in the weak coupling limit, correlations between the system and the environment (the bath) are not created if both start as initially uncorrelated thermal states. In order to do this, we will introduce a finite dimensional cut-off on $\mathcal{H}_B$ and prove the results for the truncated space, and finally proving uniform convergence in the bath size by removing the cut-off and taking the infinite dimensional limit. Let $\hat{P}_k$ denote the projection onto a finite dimensional Hilbert Space $\mathcal{H}_{B,k} \subset \mathcal{H}_B$. Furthermore, assume that $\mathcal{H}_{B,1} \subset \mathcal{H}_{B,2} \subset \mathcal{H}_{B,3} \dots$ and that $\lim_{k\to\infty} \mathcal{H}_{B,k} = \mathcal{H}_B$. For concreteness (although not strictly necessary), one could let $\hat{P}_n = \sum_{l=0}^{k} |E_l\rangle\langle E_l|$ where $|E_0\rangle, |E_1\rangle, |E_2\rangle, \dots$ are the eigenvectors of $H_B$ ordered in increasing eigenvalue order.

We define the truncated self-adjoint Hamiltonians on $\mathcal{H}_\mathcal{B}$ as $H_B^{(k)} = \hat{P}_k H_B \hat{P}_k$ with a corresponding Gibbs state denoted by $\tau_{B,k} \in \mathcal{S}(\mathcal{H}_{B,k})$. Similarly, we construct unitaries on $\mathcal{H}_{B,k}$ by

$$U_k = \exp\left(-\mathrm{i}\Delta H_{SB}^{(k)}\right), \quad H_{SB}^{(k)} = (\mathbb{I}_S \otimes \hat{P}_k)\, H_{SB}\, (\mathbb{I}_S \otimes \hat{P}_k) \tag{4.35}$$

and define $H_{I,k} := (\mathbb{I}_S \otimes \hat{P}_k)\, H_I\, (\mathbb{I}_S \otimes \hat{P}_k)$. We recall the definition of the thermal state of the system $\tau_S \in \mathcal{S}(\mathcal{H}_S)$, which is given by

$$\tau_S = \frac{\mathrm{e}^{-\beta H_S}}{Z_S}, \quad Z_S > 0 \tag{4.36}$$

for some inverse temperature $\beta > 0$

The key lemma (which we will be using later) is the following:

**Lemma 9** (Correlations at the fixed point)**.** *Let $\alpha > 0$, $\Delta \in \mathbb{R}$ and the constant $\tilde{Z}_{SB}^{k,\alpha} = \mathrm{Tr}[(\tau_S \otimes \tau_{B,k})^\alpha]$. Then, for all $k \in \mathbb{N}^+$, we have the bound*

$$\frac{1}{2}\|U_k(\tau_S \otimes \tau_{B,k})^\alpha U_k^\dagger - (\tau_S \otimes \tau_{B,k})^\alpha\|_1 \leq \tilde{Z}_{SB}^{k,\alpha}\alpha\beta\sqrt{\lambda\|H_{I,k}\|}, \tag{4.37}$$

*where $\tau_S$, $\tau_{B,k}$ are thermal states at inverse temperatures $\beta_S$, $\beta_{B,k}$ respectively, and $\|\cdot\|_1$, $\|\cdot\|$ is the one-norm and operator norm respectively.*

*Proof.* The result is a consequence of mean energy conservation under the unitary transformation $U_k$ and Pinsker's inequality.

Define the shorthand notation $\tilde{\tau}_{SB}^{k,\alpha} = U_k(\tau_S \otimes \tau_{B,k})^\alpha U_k^\dagger / \tilde{Z}_{SB}^{k,\alpha} \in \mathcal{S}(\mathcal{H}_S \otimes \mathcal{H}_{B,k})$ and $\tilde{Z}_{SB}^{k,\alpha} := \tilde{Z}_S^\alpha \tilde{Z}_B^{k,\alpha}$, $\tilde{Z}_S^\alpha := \mathrm{Tr}[\tau_S^\alpha]$, $\tilde{Z}_B^{k,\alpha} := \mathrm{Tr}[\tau_{B,k}^\alpha]$. By direct evaluation of the relative entropy,

$$D\left(\tilde{\tau}_{SB}^{k,\alpha}\middle\|\frac{(\tau_S \otimes \tau_{B,k})^\alpha}{\tilde{Z}_{SB}^{k,\alpha}}\right)/\beta = \alpha\mathrm{Tr}[H_S\tilde{\tau}_S^{k,\alpha}] + \alpha\mathrm{Tr}[H_B^{(k)}\tilde{\tau}_{B,k}^\alpha] - \beta^{-1}S\left(\frac{\tau_S^\alpha \otimes \tau_{B,k}^\alpha}{\tilde{Z}_{SB}^{k,\alpha}}\right) + \beta^{-1}\ln(\tilde{Z}_{SB}^{k,\alpha}), \tag{4.38}$$

where we have used unitary invariance of the von Neumann entropy $S(\cdot)$. Thus since

$$0 = D\left(\frac{(\tau_S \otimes \tau_{B,k})^\alpha}{\tilde{Z}_{SB}^{k,\alpha}} \middle|\middle| \frac{(\tau_S \otimes \tau_{B,k})^\alpha}{\tilde{Z}_{SB}^{k,\alpha}}\right)/\beta \tag{4.39}$$

$$0 = \mathrm{Tr}[\frac{H_S \tau_S^\alpha}{\tilde{Z}_S^\alpha}] + \mathrm{Tr}[\frac{H_B^{(k)} \tau_{B,k}^\alpha}{\tilde{Z}_B^{k,\alpha}}] - (\alpha\beta)^{-1} S\left(\frac{\tau_S^\alpha \otimes \tau_{B,k}^\alpha}{\tilde{Z}_{SB}^{k,\alpha}}\right) + (\alpha\beta)^{-1} \ln(\tilde{Z}_{SB}^{k,\alpha}), \tag{4.40}$$

we conclude

$$D\left(\tilde{\tau}_{SB}^{k,\alpha} || \frac{(\tau_S \otimes \tau_{B,k})^\alpha}{\tilde{Z}_{SB}^{k,\alpha}}\right)/(\alpha\beta) = \mathrm{Tr}[H_S \tilde{\tau}_S^{k,\alpha}] + \mathrm{Tr}[H_B^{(k)} \tilde{\tau}_B^{k,\alpha}] - \mathrm{Tr}[\frac{H_S \tau_S^\alpha}{\tilde{Z}_S^{k,\alpha}}] - \mathrm{Tr}[\frac{H_B^{(k)} \tau_{B,k}^\alpha}{\tilde{Z}_B^{k,\alpha}}]. \tag{4.41}$$

Energy conservation implies

$$\mathrm{Tr}\left[\frac{H_{SB}^{(k)} (\tau_S \otimes \tau_{B,k})^\alpha}{\tilde{Z}_{SB}^{k,\alpha}}\right] = \mathrm{Tr}[H_{SB}^{(k)} \tilde{\tau}_{SB}^{k,\alpha}]. \tag{4.42}$$

Combining Eqs. (4.42), (4.41) we achieve

$$D\left(\tilde{\tau}_{SB}^{k,\alpha} \middle|\middle| \frac{(\tau_S \otimes \tau_{B,k})^\alpha}{\tilde{Z}_{SB}^{k,\alpha}}\right) = \alpha\beta \mathrm{Tr}\left[\lambda H_{I,k}\left(\tilde{\tau}_{SB}^{k,\alpha} - \frac{(\tau_S \otimes \tau_{B,k})^\alpha}{\tilde{Z}_{SB}^{k,\alpha}}\right)\right]. \tag{4.43}$$

Pinsker's inequality states that for any two density matrices $\rho$, $\sigma$,

$$D(\rho||\sigma) \geq \frac{1}{2}\|\rho - \sigma\|_1^2. \tag{4.44}$$

It follows from it, and from Eq. (4.43) that,

$$\begin{aligned}
\|U_k(\tau_S \otimes \tau_{B,k})^\alpha U_k^\dagger - (\tau_S \otimes \tau_{B,k})^\alpha\|_1 &\leq \tilde{Z}_{SB}^{k,\alpha} \alpha\beta \sqrt{2\,\mathrm{Tr}[\lambda H_{I,k}\left(\tilde{\tau}_{SB}^{k,\alpha} - \frac{(\tau_S \otimes \tau_{B,k})^\alpha}{\tilde{Z}_{SB}^{k,\alpha}}\right)]} && (4.45)\\
&\leq 2\tilde{Z}_{SB}^{k,\alpha} \alpha\beta \sqrt{\sup_{\rho \in \mathcal{S}(\mathcal{H}_S \otimes \mathcal{H}_{B,k})} |\mathrm{Tr}[H_{I,k}\,\rho]|\,\lambda} && (4.46)\\
&\leq 2\tilde{Z}_{SB}^{k,\alpha} \alpha\beta \sqrt{\lambda \|H_{I,k}\|} && (4.47)
\end{aligned}$$

□

We can see from the form of this Lemma that in the weak couplig limit, in which $\lambda \to 0$, Eq. (4.37) expresses the fact that the global unitary generated by the interaction Hamiltonian obeys the key property of energy conservation Eq. (1.12). That and the fact that the reservoir is thermal are enough to establish them as part of the set of thermal operations.

## 4.4 A bound on the entropy production

The main new result of the present chapter is a tight lower bound on the change of free energy and total entropy produced within a finite time. It will be a particular example of the kind of theorem introduced in Section 4.1. We start by proving the first (and perhaps more important) part of the result in the following Lemma:

**Lemma 10.** *All Davies maps $T_t(\cdot)$, satisfy the inequality*

$$D(\rho_S(0)||\tau_S) - D(\rho_S(t)||\tau_S) \geq D\left(\rho_S(0)||\tilde{T}_t(\rho_S(t))\right), \tag{4.48}$$

*where $\tilde{T}_t(\cdot)$ is the* time-reversed *map or Petz recovery map, defined as*

$$\tilde{T}_t(\cdot) = \tau_S^{1/2} T_t^\dagger \left(\tau_S^{-1/2}(\cdot)\tau_S^{-1/2}\right)\tau_S^{1/2}, \tag{4.49}$$

*with $T_t^\dagger$ denoting the adjoint of $T_t$.*

*Proof.* We will use Lemma 9 and continuity arguments in order to show this. We will perform the calculations for the map $\mathrm{Tr}_B\left[\mathrm{e}^{-\mathrm{i}\tilde{t}H_{SB}}(\cdot)\otimes\rho_B\,\mathrm{e}^{\mathrm{i}\tilde{t}H_{SB}}\right]$ rather than $T_t(\cdot)$ itself. We will finally take the limit described in Eq. (4.34) to conclude the proof.

Noting that the relative entropy between two copies of the same state is zero, followed by using its additivity and unitarity invariance properties, we find for $\rho_S \in \mathcal{S}(\mathcal{H}_S)$,

$$D(\rho_S||\tau_S) = D(\rho_S\otimes\tau_{B,k}||\tau_S\otimes\tau_{B,k}) = D(U_k\rho_S\otimes\tau_{B,k}U_k^\dagger||U_k\tau_S\otimes\tau_{B,k}U_k^\dagger) \tag{4.50}$$

$$= D(U_k\rho_S\otimes\tau_{B,k}U_k^\dagger||\tau_S\otimes\tau_{B,k}+\sqrt{\lambda}\hat{B}_k(\lambda)) \tag{4.51}$$

where $\hat{B}_k(\lambda) := \left(U_k\tau_S\otimes\tau_{B,k}U_k^\dagger - \tau_S\otimes\tau_{B,k}\right)/\sqrt{\lambda}$.

With the identity $D(\gamma_{CD}||\zeta_{CD}) - D(\gamma_D||\zeta_D) = D\left(\gamma_{CD}||\exp(\ln\zeta_{CD} + \ln\mathbb{I}_C\otimes\zeta_D - \ln\mathbb{I}_C\otimes\zeta_D)\right)$

for bipartite states $\gamma_{CD}$, $\zeta_{CD}$, we have that

$$D(U_k\rho_S\otimes\tau_{B,k}U_k^\dagger||\tau_S\otimes\tau_{B,k}+\sqrt{\lambda}\hat{B}_k(\lambda))-D(\sigma_S||\tau_S+\sqrt{\lambda}\mathrm{Tr}_{B,k}[\hat{B}_k(\lambda)]) \tag{4.52}$$

$$=D\Bigg(U_k\rho_S\otimes\tau_{B,k}U_k^\dagger\Big|\Big|\exp\Big(\ln(\tau_S\otimes\tau_{B,k}+\sqrt{\lambda}\hat{B}_k(\lambda))$$

$$+\ln\sigma_S\otimes\mathbb{I}_{B,k}-\ln(\tau_S+\sqrt{\lambda}\mathrm{Tr}_{B,k}[\hat{B}_k(\lambda)])\otimes\mathbb{I}_{B,k}\Big)\Bigg) \tag{4.53}$$

$$\geq D\Bigg(\rho_S\Big|\Big|\mathrm{Tr}_{B,k}\Big[U_n^\dagger\exp\Big(\ln(\tau_S\otimes\tau_{B,k}+\sqrt{\lambda}\hat{B}_k(\lambda))$$

$$+\ln\sigma_S\otimes\mathbb{I}_{B,k}-\ln(\tau_S+\sqrt{\lambda}\mathrm{Tr}_{B,k}[\hat{B}_k(\lambda)])\otimes\mathbb{I}_{B,k}\Big)U_k\Big]\Bigg) \tag{4.54}$$

where $\sigma_S:=\mathrm{Tr}_{B,k}[U_k\rho_S\otimes\tau_{B,k}U_k^\dagger]$ and in the last line we have used the unitarity invariance of the relative entropy followed by the data processing inequality. Plugging Eq. (4.51) into Eq. (4.54) followed by taking the $k\to\infty$ limit, we obtain

$$D(\rho_S||\tau_S)-D(\sigma_S||\tau_S+\sqrt{\lambda}\mathrm{Tr}_B[\hat{B}(\lambda)]) \tag{4.55}$$

$$\geq D\Bigg(\rho_S\Big|\Big|\mathrm{Tr}_B\Big[U^\dagger\exp\Big(\ln(\tau_S\otimes\tau_B+\sqrt{\lambda}\hat{B}(\lambda))+\ln\sigma_S\otimes\mathbb{I}_B-\ln(\tau_S+\sqrt{\lambda}\mathrm{Tr}_B[\hat{B}(\lambda)])\otimes\mathbb{I}_B\Big)U\Big]\Bigg), \tag{4.56}$$

where we have defined $\hat{B}(\lambda):=\lim_{k\to\infty}\hat{B}_k(\lambda)$. Before continuing, we will first note the validity of Eq. (4.56). We start by showing that $\hat{B}(\lambda)$ is trace class for $\lambda\in[0,1]$. From Lemma 9 it follows

$$\|\hat{B}_k(\lambda)\|_1\leq 2\tilde{Z}_{SB}^{k,1}\beta\sqrt{\|H_{I,k}\|}, \tag{4.57}$$

for all $\lambda\in[0,1]$ with the RHS $\lambda$ independent. By definition of $\tilde{Z}_{SB}^{k,\alpha}$ , it follows that it is the partition function of a tensor product of thermal states on $\mathcal{S}(\mathcal{H}_S\otimes\mathcal{H}_{B,k})$ at inverse temperatures $\alpha\beta_S,\alpha\beta$. Since the Hamiltonians $\hat{H}_{B,1},\hat{H}_{B,2},\hat{H}_{B,3},\ldots,\hat{H}_B$ by definition have well defined thermal states (finite partition functions) for all positive temperatures, it follows that $\lim_{k\to\infty}\tilde{Z}_{SB}^{k,\alpha}<\infty$ for all $\alpha>0$. Thus noting that by definition, $\lim_{k\to\infty}\|H_{I,k}\|=\|H_I\|$ and that $H_I$, is a bounded operator, it follows that

$$\|\hat{B}(\lambda)\|_1=\lim_{k\to\infty}\|\hat{B}_k(\lambda)\|_1=2\tilde{Z}_{SB}^{\infty,1}\beta\sqrt{\|H_I\|}<\infty, \tag{4.58}$$

where we have set $\alpha = 1$. Thus since $\tau_S + \sqrt{\lambda}\mathrm{Tr}_B[\hat{B}(\lambda)]$ is finite dimensional and Hermitian, and the eigenvalues of finite dimensional Hermitian matrices are continuous in their entries [145, 102], it follows, since $\tau_S$ has full support, that there exists $0 < \lambda^* \leq 1$ such that for all $\lambda \in [0, \lambda^*]$, $\tau_S + \sqrt{\lambda}\mathrm{Tr}_B[\hat{B}(\lambda)]$ has full support. Thus for all $\lambda \in [0, \lambda^*]$, the RHS of Eq. (4.56) is upper bounded by a finite quantity uniformly in $k \to \infty$ and thus since relative entropies are non-negative by definition, Eq. (4.56) is well defined for all $\lambda \in [0, \lambda^*]$.

We now set $\Delta$ appearing in $U$ to $\Delta = t/\lambda^2$ followed by taking the limit $\lambda \to 0^+$ while keeping $t$ fixed in Eq. (4.56) thus achieving

$$D(\rho_S||\tau_S) - D(T_t(\rho_S)||\tau_S) \geq D\Big(\rho_S\Big|\Big|\mathrm{Tr}_B\big[U^\dagger T_t(\rho_S) \otimes \tau_B U\big]\Big), \tag{4.59}$$

where we have used that by definition, $T_t(\cdot) = \lim_{\lambda\to 0^+} \mathrm{Tr}_B[U(\cdot) \otimes \tau_B U^\dagger]$.

We now proceed to calculate the Petz recovery map for the map $T_t(\cdot)$. The adjoint map is $\mathrm{Tr}_B[\tau_B^{1/2} U^\dagger((\cdot) \otimes \mathbb{I}_B) U \tau_B^{1/2}]$. Hence from the definition in Eq. (4.3) it follows that the Petz recovery map for $T_t(\cdot)$ is

$$\tilde{T}_t(\cdot) := \tau_S^{1/2}\mathrm{Tr}_B\left[\tau_B^{1/2} U^\dagger \left(\tau_S^{-1/2}(\cdot)\tau_S^{-1/2} \otimes \mathbb{I}_B\right) U \tau_B^{1/2}\right]\tau_S^{1/2}. \tag{4.60}$$

Similarly to before, we define a traceless, self adjoint operator

$$\tilde{B} = \tilde{B}(\lambda) := \left(U\tau_S^{1/2} \otimes \tau_B^{1/2} U^\dagger - \tau_S^{1/2} \otimes \tau_B^{1/2}\right)/\sqrt{\lambda}. \tag{4.61}$$

In analogy with the reasoning which led to Eq. (4.58), it follows from Lemma 9 that $\|\tilde{B}(\lambda)\|_1 = \lim_{k\to\infty}\|\tilde{B}_k(\lambda)\|_1 = 2\tilde{Z}_{SB}^{\infty,1/2}{}^{1/2}\beta\sqrt{\|H_I\|} < \infty$, for all $\lambda \in [0, 1]$. For general $U = \exp(-\mathrm{i}\Delta H_{SB})$, we can now write

$$\tau_S^{1/2}\mathrm{Tr}_B\left[\tau_B^{1/2} U^\dagger \left(\tau_S^{-1/2}(\cdot)\tau_S^{-1/2} \otimes \mathbb{I}_B\right) U \tau_B^{1/2}\right]\tau_S^{1/2} \tag{4.62}$$

$$= \mathrm{Tr}_B\left[\left(U^\dagger \tau_S^{1/2} \otimes \tau_B^{1/2} + \sqrt{\lambda} U^\dagger \tilde{B}\right)\left(\tau_S^{-1/2}(\cdot)\tau_S^{-1/2} \otimes \mathbb{I}_B\right)\left(\tau_S^{1/2} \otimes \tau_B^{1/2} U + \sqrt{\lambda}\tilde{B}U\right)\right] \tag{4.63}$$

$$= \mathrm{Tr}_B[U^\dagger\left((\cdot) \otimes \tau_B\right)U] + \sqrt{\lambda}\hat{g}_1(\cdot) + \lambda\hat{g}_2(\cdot) \in \mathcal{S}(\mathcal{H}_B), \tag{4.64}$$

where

$$\hat{g}_1(\cdot) = \mathrm{Tr}_B\left[U^\dagger \tilde{B}(\tau_S^{-1/2}(\cdot) \otimes \tau_B^{1/2})U\right] + \mathrm{Tr}_B\left[U^\dagger((\cdot)\tau_S^{-1/2} \otimes \tau_B^{1/2})\tilde{B}U\right] \tag{4.65}$$

$$\hat{g}_2(\cdot) = \mathrm{Tr}_B\left[U^\dagger \tilde{B}\left(\tau_S^{-1/2}(\cdot)\tau_S^{-1/2} \otimes \mathbb{I}_B\right)\tilde{B}U\right], \tag{4.66}$$

which are well defined since they are comprised of products of bounded operators. Similarly to before, in Eq. (4.64) we now set $\Delta$ appearing in $U$ to $\Delta = t/\lambda^2$ followed by taking the limit $\lambda \to 0^+$ while keeping $t$ fixed achieving

$$\tilde{T}_t(\cdot) = \mathrm{Tr}_B[U^\dagger\left((\cdot)\otimes\tau_B\right)U] \tag{4.67}$$

where we have used Eq. (4.60). Hence substituting Eq. (4.65) in to Eq. (4.59) and noting the equations holds for all states $\rho_S \in \mathcal{S}(\mathcal{H}_S)$, we conclude the proof. □

Eq. 4.49 shows that Conjecture 1 from [108] is indeed true for Davies maps. Again, this inequality is known to not be true for general quantum maps, and this presents one of the first examples for which it is.

### 4.4.1 Quantum detailed balance and Petz recovery map

For Lemma 10 to hold, only properties 1) and 4) are required. In addition, we will find below that there is a connection between property 5) and the Petz recovery map which we will now explain. Essentially, a quantum dynamical semi-group with no unitary part $M_t$ which obeys QDB has a Petz recovery map $\tilde{M}_t$ which is equal to the map itself $\tilde{M}_t = M_t$ (See Lemma 11).

The classical definition of detailed balance, in terms of the transition probabilities $p(j|i)$ of a classical Master equation, implies that, at equilibrium, a particular jump between energy levels $E_i \to E_j$ has the same total probability as the opposite jump $E_j \to E_i$, such that $p(j|i)\frac{e^{-\beta E_i}}{Z_S} = p(i|j)\frac{e^{-\beta E_j}}{Z_S}$. The condition in Eq. (4.25) is then the most natural quantum generalization of that. In that sense, QDB can be understood as the fact that a particular thermalization process coincides with its own time-reversed map, which is defined as in Eq. (4.49). There are a number of alternative notions of quantum detailed balance in the literature, but in Appendix A.2 we show that in the context of Davies maps all of these turn out to be equivalent, and we hence can freely take the one given in Eq. (4.25).

#### Main result

Before the main theorem, we will write a Lemma that shows the explicit relation between QDB and the Petz recovery map. For the sake of generality, we show the that the result is true for any fixed point $\Omega$ with full support, with respect to which detailed balance is defined. We remind the reader, that a dynamical semigroup $M_t(\cdot)$ is a one parameter family of CPTP maps with a generator consisting of a unitary part $\theta(\cdot) = -[\hat{H}_{\text{eff}}, \cdot]$, and a dissipative part called a Lindbladian, $\mathcal{L}(\cdot)$, such that all together we have

$$M_t(\cdot) = \mathrm{e}^{ti\theta + t\mathcal{L}}(\cdot) \tag{4.68}$$

.

**Lemma 11** (Dissipative Recovery map)**.** *A quantum dynamical semigroup $M_t(\cdot)$ with no unitary part, $\theta = 0$, and Lindbladian $\mathcal{L}$ satisfying quantum detailed balance (Eq.* (4.25)*) for the state $\Omega$ with full rank, is equal to its corresponding Petz recovery map, namely,*

$$M_t(\cdot) = \tilde{M}_t(\cdot), \tag{4.69}$$

*where*

$$\tilde{M}_t(\cdot) = \Omega^{1/2} M_t^{\dagger}(\Omega^{-1/2} \cdot \Omega^{-1/2})\Omega^{1/2}. \tag{4.70}$$

*Proof.* Again the property of quantum detailed balance reads

$$\langle A, \mathcal{L}^{\dagger}(B)\rangle_{\Omega} = \langle \mathcal{L}^{\dagger}(A), B\rangle_{\Omega} \tag{4.71}$$

for all $A, B \in \mathbb{C}^{n\times n}$, where $\mathcal{L}^{\dagger}$ is the adjoint Lindbladian, and the scalar product is

$$\langle A, B\rangle_{\Omega} := \mathrm{Tr}[\Omega^{1/2} A^{\dagger} \Omega^{1/2} B]. \tag{4.72}$$

Because Eq. (4.71) holds for all $A, B \in \mathbb{C}^{n\times n}$, Eq. (4.71) implies that [134]

$$\mathcal{L}(\cdot) = \Omega^{1/2} \mathcal{L}^{\dagger}(\Omega^{-1/2} \cdot \Omega^{-1/2})\Omega^{1/2}. \tag{4.73}$$

Eq. (4.71) automatically implies that any power of the generator also obeys the same relation, that is, $\forall\, l \in \mathbb{N}^{+}$

$$\begin{aligned}
\langle A, \mathcal{L}^{\dagger l}(B)\rangle_{\Omega} &= \langle A, \Omega^{-1/2}\mathcal{L}(\Omega^{1/2} \ldots \Omega^{-1/2}\mathcal{L}(\Omega^{1/2} B \Omega^{1/2})\Omega^{-1/2} \ldots \Omega^{1/2})\Omega^{-1/2}\rangle_{\Omega} &(4.74)\\
&= \langle A, \Omega^{-1/2}\mathcal{L}^{l}(\Omega^{1/2} B \Omega^{1/2})\Omega^{-1/2}\rangle_{\Omega} &(4.75)\\
&= \langle \mathcal{L}^{\dagger\, l}(A), B\rangle_{\Omega}, &(4.76)
\end{aligned}$$

where in the first line we use Eq. (4.73) $n$ times and the 2nd line follows from the definition of the adjoint map. Hence we can also write

$$\mathcal{L}^l(\cdot) = \Omega^{1/2}\mathcal{L}^{\dagger\, l}(\Omega^{-1/2}\cdot\Omega^{-1/2})\Omega^{1/2}. \tag{4.77}$$

The semigroup can be written as $M_t(\cdot) = e^{\mathcal{L}t}(\cdot)$. Its adjoint semigroup is given by $e^{\mathcal{L}^\dagger t}$ and hence the Petz recovery map is (see Eq.(4.3))

$$\tilde{M}_t(\cdot) = \Omega^{1/2}e^{\mathcal{L}^\dagger t}(\Omega^{-1/2}\cdot\Omega^{-1/2})\Omega^{1/2}. \tag{4.78}$$

Since, $\tilde{M}_t(\cdot) = \Omega^{1/2}\left(\sum_{l=0}^{\infty}(t\mathcal{L})^{\dagger l}(\Omega^{-1/2}\cdot\Omega^{-1/2})/(l!)\right)\Omega^{1/2}$, Eq. (4.78) together with Eq. (4.77), means that $\tilde{M}_t(\cdot) = M_t(\cdot)$.

□

When the generator is time-independent and $\theta = 0$, we thus have from Theorem 11 that the combination of a map for a time $t$ and its recovery map is equivalent to applying the map for a time $2t$. That is $\tilde{M}_t(M_t(\cdot)) = M_{2t}(\cdot)$. This means we can write Eq. (4.48) in a particularly simple form, as captured by the theorem below.

Putting all of the ingredients together we finish with the central result of the chapter, which holds for Davies maps with no unitary part.

**Theorem 22.** *Assume conditions in Section 4.3.1 hold and $T_t(\cdot)$ satisfies quantum detailed balance (Eq. (4.25)) and has zero unitary part, $\theta = 0$. Then $T_t(\cdot)$ satisfies the inequality*

$$F_\beta((\cdot)) - F_\beta(T_t(\cdot)) \geq D\left((\cdot)\middle|\middle|T_{2t}(\cdot)\right), \quad t \geq 0. \tag{4.79}$$

*Proof.* Direct consequence of Lemmas 11 and 10, and of the definition of free energy. □

In order to introduce the unitary part, the next Lemma builds on Theorem 11 to extend it to the case in which the dynamical semigroup also includes it.

**Lemma 12** (Dissipative and unitary Recovery map)**.** *Let $M_t(\cdot)$ be a quantum dynamical semigroup with unitary part $\theta$ and Lindbladian $\mathcal{L}$ which: 1) satisfying quantum detailed balance (Eq. (4.25)) for the state $\Omega$ with full rank and 2) commute, $\theta(\mathcal{L}(\cdot)) = \mathcal{L}(\theta(\cdot))$. Then, $M_t(\cdot)$ has a Petz recovery map $\tilde{M}(\cdot)$ which is a dynamical semigroup with unitary part $-\theta$ and Lindbladian $\mathcal{L}$. Namely, if*

$$M_t(\cdot) = \mathrm{e}^{ti\theta + t\mathcal{L}}(\cdot), \tag{4.80}$$

*satysfying 1) and 2), then*

$$\tilde{M}_t(\cdot) = \mathrm{e}^{-ti\theta + t\mathcal{L}}(\cdot). \tag{4.81}$$

*Proof.* We just need to note two facts:

- The Petz recovery map of a unitary map $U(\cdot)U^\dagger$ that had fixed point $\Omega$ is $U^\dagger(\cdot)U$.
- The Petz recovery map of a composition of two maps with the same fixed point, is equal to the composition of the Petz recovery maps of the individual maps, i.e. $\widetilde{\Gamma_1 \circ \Gamma_2} = \tilde{\Gamma}_2 \circ \tilde{\Gamma}_1$ (this is one of the key properties listed in [108]).

We hence can write the recovery map of $M_t(\cdot)$ as

$$\tilde{M}_t(\rho_S) = e^{t\mathcal{L}}(e^{iH_{\text{eff}}t}\rho_S e^{-iH_{\text{eff}}t}) = e^{iH_{\text{eff}}t} e^{t\mathcal{L}}(\rho_S) e^{-iH_{\text{eff}}t}. \tag{4.82}$$

The only difference between $M_t$ and $\tilde{M}_t$ is the change of sign in the time of the unitary evolution. The recovery map is then made up of the dissipative part evolving forwards, and the unitary part evolving backwards in time. □

While the absence of a unitary part is a limitation of Theorem 22, we now stress that even for the general Davies maps the following remark holds if we only take into account the dissipative part in the lower bound.

**Remark 23** (When $\theta \neq 0$)**.** *Due to properties 3), 5) of Section 4.3 satisfied by Davies maps, and the unitary invariance of the relative entropy (i.e. $D(U \cdot U^\dagger || U \cdot U^\dagger) = D(\cdot||\cdot)$), it follows*

$$D((\cdot)||\tau_S) - D(T_t(\cdot)||\tau_S) = D((\cdot)||\tau_S) - D(\mathrm{e}^{t\mathcal{L}}(\cdot)||\tau_S), \tag{4.83}$$

*and thus the LHS of Eq.* (4.79) *is the same even when a non zero unitary part is included. Furthermore, we note that the canonical form of Davies maps have $\theta(\mathcal{L}(\cdot)) = \mathcal{L}(\theta(\cdot))$ by definition and thus, due to Lemma 12, even when $\theta \neq 0$, we have that*

$$D((\cdot)||\tilde{T}_t(T_t(\cdot))) = D((\cdot)||\mathrm{e}^{2t\mathcal{L}}(\cdot)), \tag{4.84}$$

*which is the r.h.s. of Eq.* (4.79)*. Thus applying Theorem 10, we have*

$$D((\cdot)||\tau_S) - D(T_t(\cdot)||\tau_S) = D((\cdot)||\tau_S) - D(\mathrm{e}^{t\mathcal{L}}(\cdot)||\tau_S) \geq D((\cdot)||\mathrm{e}^{2t\mathcal{L}}(\cdot)), \tag{4.85}$$

*for any $\theta$.*

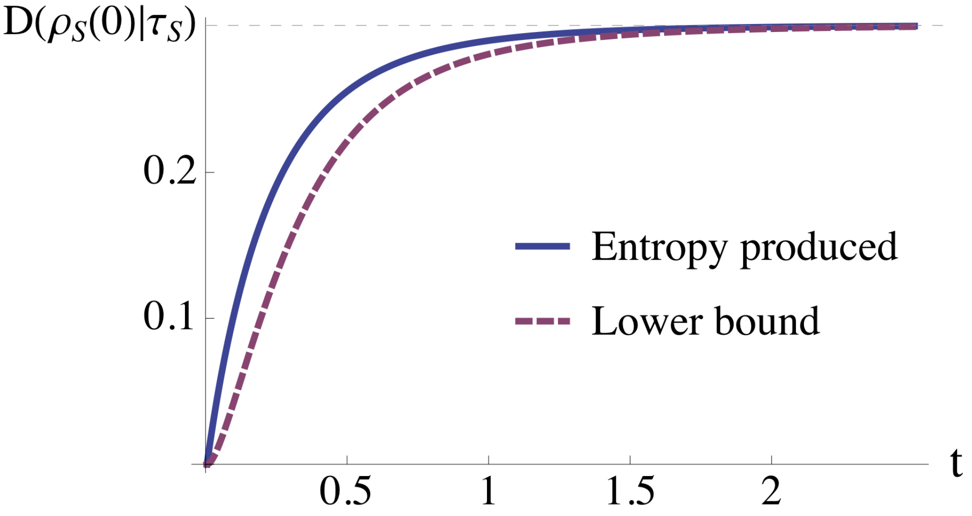

Figure 4.1: A generic example of the inequality in Theorem 22 for a Davies map on a qutrit given in [154]. The initial state is chosen at random from all possible qutrit mixed states, and the thermal state has populations $q_\beta = (0.6, 0.3, 0.1)$. The solid (blue) curve is the amount of entropy produced $\beta F_\beta(\rho(0)) - \beta F_\beta(\rho(t))$ and the dashed (purple) the lower bound $D(\rho_S(0)||\rho_S(2t))$. It can be seen how the lower bound at $t = 0$ starts at zero, and how for large times the two curves quickly converge to the total amount of entropy produced $D(\rho_S(0)||\tau_S)$. Other numerical examples for different initial states far enough from thermal show very similar behavior.

We note that in order to obtain the last two results, in addition to assuming detailed balance, condition 5), we have also used condition 2).

In Fig. 4.1 we show a simple example of the inequality for the case of Davies maps applied on a qutrit. Eq. (4.79) is tight at $t = 0$ and also in the large time limit, as long as condition 6) is satisfied. In this limit, the total entropy that has been produced is equal to $\frac{1}{\beta} D(\rho(0)|\tau_S)$, which both sides of the inequality approach as $\rho_S \to \tau_S$.

On the other hand, for very short times, the lower bound becomes trivial. In particular, in Appendix A.3 we show what both sides of the inequality tend to in the limit of infinitesimal time transformations. The entropy production becomes a *rate*, and the lower bound to it approaches 0.

Non-trivial lower bounds on the rate of entropy production, in the form of log-Sobolev inequalities [100] can be used to derive bounds on the time it takes to converge to equilibrium for particular instances of Davies maps. Hence, given that Theorem 22 holds for all dissipative Davies maps, and holds also for those that do not efficiently reach thermal equilibrium (or that do not reach it at all for some initial states), the fact that the lower bound vanishes for infinitesimal times is not surprising.

Recall that the factor of 2 in Eq. (4.79) is a consequence of the observation that the Petz recovery map is equal to the map itself. A natural question is then, *is the factor* 2 *fundamental?* We show that this is indeed the case with the following Theorem.

**Theorem 24.** *[Tightness of the entropy production bound] The largest constant $k \geq 0$ such that*

$$F_\beta(\rho_S(0)) - F_\beta(\rho_S(t)) \geq \frac{1}{\beta} D\left(\rho_S(0) \big|\big| \rho_S(k\, t)\right) \tag{4.86}$$

*holds for all Davies maps, is $k = 2$.*

*Proof.* We show the inequality is violated for any $k > 2$ by finding a simple family of Davies maps for which the violation is proven analytically.

Let us take the general form of a Davies map on a qubit [154], and act on a state with initial density matrix $\rho$ without coherence in energy $\rho(0) = \mathrm{diag}(p(0), 1-p(0))$, and with a corresponding thermal state $\tau = \mathrm{diag}(q, 1-q)$. The time evolution of the Davies map is only that of the populations (as no coherence in the energy eigenbasis is created), and it takes the general form

$$\begin{pmatrix} p(t) \\ 1-p(t) \end{pmatrix} = \begin{pmatrix} 1-a_t & a_t \frac{q}{1-q} \\ a_t & 1-a_t\frac{q}{1-q} \end{pmatrix} \begin{pmatrix} p(0) \\ 1-p(0) \end{pmatrix}, \tag{4.87}$$

where $a_t = (1-q)(1-e^{-At})$ for some $A > 0$. Let us now define the function

$$g(t,k) := \beta F_\beta(\rho_S(0)) - \beta F_\beta(\rho_S(t)) - D\left(\rho_S(0) \big|\big| \rho_S(k\, t)\right), \tag{4.88}$$

and the variable $x := e^{-At}$. One can show, after some algebra, that for the time evolution of Eq. (4.87)

$$\begin{aligned} g(x,k) = \big[(q-1) + x(p(0)-q)\big] \log\left(1 + x\frac{q-p(0)}{1-q}\right) - [q + x(p(0)-q)] \\ +(1-p(0))\log\left(1 + x^k \frac{q-p(0)}{1-q}\right) + p(0)\log\left(1 + x^k\frac{p(0)-q}{q}\right). \end{aligned} \tag{4.89}$$

For large $t$, $x$ will be arbitrarily small and hence we can expand the logarithms up to leading order in $x$. The zeroth and first order terms in $x$ cancel out, and we obtain

$$g(x,k) = \frac{-1}{2q(1-q)} x^2 (p(0)-q)^2 + \frac{1}{q(1-q)} x^k (p(0)-q)^2 + \mathcal{O}(x^3). \tag{4.90}$$

We see that if $k > 2$, for sufficiently large time, the $k$-th order term will be very small compared to the $x^2$ one, which is always negative. For $k = 2$ we have

$$g(x,2) = \frac{1}{2q(1-q)} x^2 (p(0)-q)^2 + \mathcal{O}(x^3), \tag{4.91}$$

such that the leading order is always positive. This completes the proof.

□

See Fig. 4.2 for more details. This means that Eq. (4.79) is the strongest constraint of its kind that Davies maps obey, and it hence sets an optimal relation between how much the free energy and the systems state at a later time change during a thermalization process.

## 4.5 Outlook

One of the main features in the study of dynamical thermalisation processes, such as Davies maps, is quantum detailed balance (QDB). By using tools from quantum information theory, we have shown in this chapter how the entropy produced after a time $t$ is lower bounded by how well one can *recover* the initial $\rho_S(0)$ state from the state $\rho_S(t)$ via a recovery map. We then show that, due to QDB, the best way to perform the recovery is to evolve *forward* in time an amount $t$ to the state $\rho_S(2t)$. What's more, if one time evolves $\rho_S(t)$ for time $t' < t$, a worse bound is generated, while if one evolves for $t' > t$, the bound is not true for all Davies maps; thus showing that the connection between reversibility and recoverability suggested by QDB leads to tight dynamical bounds.

One of the important questions regarding Davies maps is how fast they converge to equilibrium. There have been several approaches to this question, mostly inspired by their classical analogues, which include the computation of the spectral gaps [10, 174, 176] or the logarithmic-Sobolev inequalities [100, 177]. In particular we note that the latter take the form of upper bounds on distance measures between $\rho_S(t)$ and the thermal state. Likewise Eq. (4.79) can

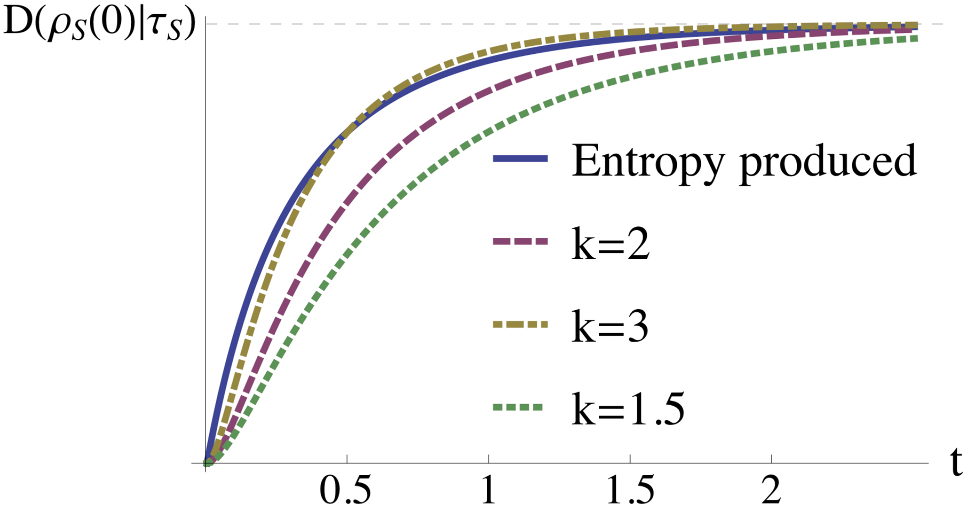

Figure 4.2: Example plots for Theorem 24 for the Davies map for qutrits from [154]. The solid (blue) curve is the amount of entropy produced $\beta F_\beta(\rho(0)) - \beta F_\beta(\rho(t))$ (LHS of Eq. (4.86)) while the dashed lines correspond to $D(\rho(0)||\rho(kt))$ (r.h.s. of Eq. (4.86)) for different $k$. The initial and thermal states are the same as those of Fig. 4.1. We see that when the constant $k$ is greater than 2 the bound does not hold any more, showing that the $k = 2$ case is indeed special. For $k < 2$ the bound holds intuitively (given that it holds for $k = 2$), but results in a worse bound. This shows that the constraint set by Eq. (4.79) reflects a special feature of how Davies maps thermalize. Moreover, we see that a $k > 2$ would predict (incorrectly) a faster thermalisation rate, thus confirming that Eq. (4.79) is an implicit universal bound on the rate of thermalisation for Davies maps.

be re-arranged to give an upper bound in terms of the relative-entropy to the Gibbs state, $D(\rho_S(t)||\tau_S) \leq D(\rho_S(0)||\tau_S) - D\left(\rho_S(0)\middle|\middle|\rho_S(2t)\right)$. It would be interesting to know if the bound of Eq. (4.79), for *primitive* Davies Maps, i.e. the dynamics converge to a unique fixed point, contains information about their asymptotic convergence. For instance, one could look at how fast is the inequality saturated in particular cases.

Another potential application of the results of the chapter in open quantum systems, is to use a tightened data processing inequality to find when *information backflow* occurs in non-Markovian dynamics [106].

The condition of detailed balance is ubiquitous in thermalization processes, and in particular, current algorithms for simulating thermal states on a quantum computer, such as the quantum Metropolis algorithm [175], obey it, which makes it all the more interesting. As such, the connection established here between the Petz recovery map and QDB, may have further implications for both thermodynamics and information theory.

## 4.6 Summary

At the beginning of this chapter we introduced two very important concepts:

- Recovery map: given a quantum CPTP map, we define this as another map which when applied to a particular pair of states recovers them well, as quantified by Petz's theorem and subsequent generalizations. How "well" a particular evolution can be recovered is directly related to how big the decrease of relative entropy is.
- Entropy production: this key quantity represents the change of entropy of both the system and the heat bath involved, added together without considering correlations. In the context of a weak interaction with a thermal reservoir, we saw that we can link the entropy of the bath with the heat (or change of energy of the bath), which lead to identifying a decrease of relative entropy with the entropy production. We also saw explicitly how this entropy production is related to the correlations between system and bath, and with the change of state of the bath.

These two notions have in common the appearance of the decrease of relative entropy. We use this, and the connection between quantum detailed balance and the definition of recovery map, to show a bound on entropy production at time $t$ in terms of the state of the system at times 0 and $2t$ for Markovian evolutions in which a system is weakly coupled to a large reservoir. These maps usually go under the name of Davies maps. This way we link the entropy production with the change of state, and through our main result we highlight how quantum information ideas can be useful in a simple scenario, while also give physical meaning to the quantum information results.

# Appendix A

# Technical proofs

## A.1 Proofs of Lemma 7 on unitaries with translation invariance

We here give a proof of Lemma 7 from Chapter 3.

**Lemma 13.** *A map $\Gamma_{SBW}$ obeys the three constraints above (unitarity, energy conservation, and independence on the state of the weight) if and only if there is an arbitrary system-bath unitary $V_{SB}$ such that the global unitary on system, bath and weight can be written as*

$$\begin{aligned} U_{SBW} &= e^{i(H'_S+H_B)\otimes\Delta_W}\,(V_{SB}\otimes\mathbb{I}_W)\,e^{-i(H_S+H_B)\otimes\Delta_W} \\ &= \int dt\, A_{SB}(t)\otimes|t\rangle\langle t|\ , \end{aligned}$$

*where we define the family of unitaries*

$$A_{SB}(t) = e^{it(H'_S+H_B)}V_{SB}\,e^{-it(H_S+H_B)}\ .$$

*Proof.* Most of the following arguments do not exploit the system-bath partition. Hence, in order to simplify the expressions, we jointly call them "composite" $C = SB$, as in $H_C = H_S+H_B$ or $\rho_{CW} = \rho_{SBW}$. We now use the assumptions on the global unitary $U_{CW}$.

We start by imposing the translation invariance of the map. For this, we note that the only operators which commute with $\Delta_W$ are the functions of itself, $f(\Delta_W)$, and that a complete basis of these functions are the imaginary exponentials $e^{i\mathcal{E}\Delta_W}$. Hence, the condition $[U_{CW},\Delta_W] = 0$ implies

$$U_{CW} = \int d\mathcal{E}\, A_C(\mathcal{E})\otimes e^{i\mathcal{E}\Delta_W}\ , \tag{A.1}$$

where $A_C(\mathcal{E})$ with $\mathcal{E} \in \mathbb{R}$ is a one-parameter family of operators.

Next, we impose *energy conservation*

$$U_{CW}(H_C + H_W) = (H'_C + H_W)U_{CW} \ . \tag{A.2}$$

Note that the equation $[H_W, \Delta_W] = i$ implies that $[H_W, e^{i\mathcal{E}\Delta_W}] = -\mathcal{E}\, e^{i\mathcal{E}\Delta_W}$ and

$$\int d\mathcal{E}\, \big(A_C(\mathcal{E})H_C - H'_C A_C(\mathcal{E}) + \mathcal{E} A_C(\mathcal{E})\big) \otimes e^{i\mathcal{E}\Delta_W} = 0 \ .$$

This and the linear independence of the operators $e^{i\mathcal{E}\Delta_W}$ gives

$$H'_C A_C(\mathcal{E}) = A_C(\mathcal{E})\, (H_C + \mathcal{E}) \ , \tag{A.3}$$

for all $\mathcal{E} \in \mathbb{R}$. If we translate this equation to Fourier space using

$$A_C(\mathcal{E}) = \frac{1}{2\pi} \int dt\, e^{-i\mathcal{E}t} A_C(t) \ , \tag{A.4}$$

we obtain

$$H'_C A_C(t) = A_C(t)H_C - i\, \partial_t A_C(t) \ . \tag{A.5}$$

The solutions of this differential equation are given simply by

$$A_C(t) = \mathrm{e}^{itH'_C} V_C\, \mathrm{e}^{-itH_C} \ , \tag{A.6}$$

where $V_C$ is arbitrary.

Finally, we impose *unitarity* $U_{CW}U^\dagger_{CW} = \mathbb{I}_{CW}$. That is

$$\mathbb{I}_C \otimes \mathbb{I}_W = \int d\mathcal{E}' d\mathcal{E}\, A_C(\mathcal{E}')A^\dagger_C(\mathcal{E}) \otimes \mathrm{e}^{i(\mathcal{E}'-\mathcal{E})\Delta_W} \ . \tag{A.7}$$

Using the linear independence of $\mathrm{e}^{i\mathcal{E}\Delta_W}$ we obtain

$$\int d\mathcal{E}\, A_C(\mathcal{E})A^\dagger_C(\mathcal{E} + E) = \mathbb{I}_C\, \delta(E) \ , \tag{A.8}$$

for all $E \in \mathbb{R}$. If we translate this equation to Fourier space using Eq. (A.4) we get $A_C(t)A^\dagger_C(t) = \mathbb{I}_C$, which implies $V_C V^\dagger_C = \mathbb{I}_C$.

Substituting Eq. (A.6) into Eq. (A.1) gives

$$\begin{aligned} U_{CW} &= \int dE\, dt\, \mathrm{e}^{-iEt} A_C(t) \otimes \mathrm{e}^{iE\Delta_W} \\ &= \int dt\, A_C(t) \otimes |t\rangle\langle t| \ . \end{aligned} \tag{A.9}$$

An equivalent form can be obtained by using the eigen-projectors of $H_C = \int d\mathcal{E}\,\mathcal{E}\,P_{\mathcal{E}}$ and $H'_C = \int d\mathcal{E}'\mathcal{E}'P_{\mathcal{E}'}$. That is

$$\begin{aligned} U_{CW} &= \int d\mathcal{E}'d\mathcal{E}\,dE\,dt\,\mathrm{e}^{i(\mathcal{E}'-\mathcal{E}-E)t}\,[P_{\mathcal{E}'}V_C P_{\mathcal{E}}]\otimes \mathrm{e}^{iE\Delta_W} \\ &= \int d\mathcal{E}'d\mathcal{E}\,[P_{\mathcal{E}'}V_C P_{\mathcal{E}}]\otimes \mathrm{e}^{i(\mathcal{E}'-\mathcal{E})\Delta_W} \qquad (A.10) \\ &= \mathrm{e}^{iH'_C\otimes\Delta_W}A_C\,\mathrm{e}^{-iH_C\otimes\Delta_W}\ . \qquad (A.11) \end{aligned}$$

If the spectra of $H_C$ and $H'_C$ are discrete, $H_C = \sum_c \mathcal{E}_c|c\rangle\langle c|$ and $H'_C = \sum_{c'} \mathcal{E}_{c'}|c,\rangle\langle c,|$, then we can write the above as

$$U_{CW} = \sum_{c',c} |c'\rangle\langle c'|V_C|c\rangle\langle c| \otimes \mathrm{e}^{i(\mathcal{E}_{c'}-\mathcal{E}_c)\Delta_W}\ . \qquad (A.12)$$

We note that there is no constraint on $V_C$ beyond the fact that it is a unitary operator.

□

## A.2 Equivalence of definitions of quantum detailed balance

Here we will clarify the following issue: the classic definition of detailed balance as it was first formulated in [9] does not correspond to the one we give in definition 5) and Eq. (4.25). However, we are able to show that both definitions, and a wealth of other ones such as the ones in [174], are equivalent for Davies maps.

In the literature, different nonequivalent definitions of the property of quantum detailed balance have been given. While in many places the one given is that of Eq. (4.25), an alternative definition, which can be found for instance in [12, 105] is that the Lindbladian is self-adjoint with respect to the inner product

$$\langle A, \mathcal{L}^\dagger(B)\rangle'_\Omega = \langle \mathcal{L}^\dagger(A), B\rangle'_\Omega, \qquad (A.13)$$

for all $A, B \in \mathbb{C}^{n\times n}$, where the inner product is defined as

$$\langle A, B\rangle'_\Omega = \mathrm{Tr}[\Omega A^\dagger B]. \qquad (A.14)$$

Eq. A.14 is different from that of Eq. (4.72) due to the noncommutativity of the operators. The solution to Eq (A.13) is [58]

$$\mathcal{L}(\cdot) = \Omega\mathcal{L}^\dagger(\Omega^{-1}\cdot), \qquad (A.15)$$

while the solution to Eq. (4.25) is [134]

$$\mathcal{L}(\cdot) = \Omega^{1/2}\mathcal{L}^{\dagger}(\Omega^{-1/2} \cdot \Omega^{-1/2})\Omega^{1/2}. \tag{A.16}$$

We have to re-introduce the concept of time-translation invariance, which can be thought of as equivalent to property 3) in the list above (and thus Davies maps satisfy it). For a generator $\mathcal{L}$ with fixed point $\Omega$, we define the following property, which is obeyed by Davies maps with respect to the thermal state.

**Definition 16** (Time-translation invariance w.r.t. fixed point)**.**

$$\mathcal{L}(\cdot) = \Omega^{it}\mathcal{L}\left(\Omega^{-it}(\cdot)\Omega^{it}\right)\Omega^{-it} \;\; \forall t \in \mathbb{R}. \tag{A.17}$$

This expression is analogous to that shown for general thermal operations in Lemma 2 in Chapter 1, and follows from Eq. (4.22).

We now give a simple proof of the fact that, under this condition that the map is time-translation invariant w.r.t. fixed point, the two conditions are the same.

**Theorem 25.** *For a Lindbladian operator $\mathcal{L}(\cdot)$ which obeys the property of time-translation symmetry w.r.t. a fixed point $\Omega$ of full rank (Eq.* (A.17)*), the quantum detailed balance conditions of Eq.* (A.15) *and Eq.* (A.16) *are equivalent.*

*Proof.* We rewrite both Eq. (A.15) and Eq. (A.16) in terms of their individual matrix elements in the orthonormal basis $\{|i\rangle\}$ in which $\Omega = \sum_i p_i |i\rangle\langle i|$ is diagonal. Eq. (A.15) can be written in the form

$$\langle i|\mathcal{L}(|n\rangle\langle m|)|j\rangle = \frac{p_i}{p_n}\langle i|\mathcal{L}^{\dagger}(|n\rangle\langle m|)|j\rangle \tag{A.18}$$

and Eq. (A.16) is

$$\langle i|\mathcal{L}(|n\rangle\langle m|)|j\rangle = \sqrt{\frac{p_i p_j}{p_n p_m}}\langle i|\mathcal{L}^{\dagger}(|n\rangle\langle m|)|j\rangle. \tag{A.19}$$

We can see that for each matrix element the conditions only change by the factors multiplying in front, which are different unless $\frac{p_n}{p_m} = \frac{p_i}{p_j}$.

Let us now introduce the following decomposition of operators in $\mathbb{C}^{n\times n}$ in terms of their *modes of coherence*

$$A = \sum_{\omega} A_{\omega}, \tag{A.20}$$

where $A_\omega$ is defined as

$$A_\omega = \sum_{\substack{k,l \\ \text{s.t. } \omega = \log \frac{p_k}{p_l}}} |k\rangle\langle k|A|l\rangle\langle l|. \tag{A.21}$$

The name of *modes of coherence* is due to the fact that under the action of the unitary $\Omega^{-it}$ they rotate with a different Bohr frequency, that is

$$\Omega^{-it} A_\omega \Omega^{it} = A_\omega e^{-i\omega t}. \tag{A.22}$$

If the Lindbladian has the property of time-translational invariance w.r.t. the fixed point (Eq. (A.17)), it can be shown [121, 116] that each input mode is mapped to its corresponding output mode of the same Bohr frequency $\omega$. We can write this fact as

$$\mathcal{L}(A_\omega) = \mathcal{L}(A)_\omega. \tag{A.23}$$

This means that in Eq. (A.18) and (A.19), $\langle i|\mathcal{L}(|n\rangle\langle m|)|j\rangle = 0$ unless the Bohr frequencies coincide at the input and the output, that is, when $\log \frac{p_n}{p_m} = \log \frac{p_i}{p_j}$. That is, the two conditions are nontrivial only in those particular matrix elements in which both are equivalent. $\square$

## A.3 Spohn's inequality: rate of entropy production

We give an alternative proof of a well-known result which was first shown in [165] that gives the expression for the infinitesimal rate of entropy production of a Davies map. This is stated without a proof in many standard references such as [34, 12]. Then we show in a similar way how in the infinitesimal time limit our lower bound in Theorem 22 becomes trivial.

First we need the following lemma, which proof can be found in, for instance, [43].

**Lemma 14.** *Let $\mathbb{I} \in \mathbb{C}^{n\times n}$ be the identity matrix, and $A, B \in \mathbb{C}^{n\times n}$ be matrices such that both $A$ and $A + tB$ are positive with $t \in \mathbb{R}$, we have that*

$$\log(A + tB) - \log A = t \int_0^1 \frac{1}{(1-x)A + x\mathbb{I}} B \frac{1}{(1-x)A + x\mathbb{I}} dx + \mathcal{O}(t^2) \tag{A.24}$$

With this, we can show the following:

**Theorem 26.** *Let $\mathcal{L}(\rho_S(t))$ be the generator of a dynamical semigroup, with a fixed point $\tau_S$ such that $\mathcal{L}(\tau_S)=0$. We have that the entropy production rate $\sigma(\rho_S(t))$ is given by*

$$\sigma(\rho_S(t)) := -\frac{dD(\rho_S(t)||\tau_S)}{dt} = Tr[\mathcal{L}(\rho_S(t))(\log\tau_S - \log\rho_S(t))] + Tr[\mathcal{L}(\rho_S(t))\Pi_{\rho_S(t)}] \geq 0, \quad (A.25)$$

*where $\Pi_{\rho_S(t)}$ is the projector onto the support of $\rho_S(t)$. The second term of the sum vanishes at all times for which the rate is finite.*

*Proof.* The last inequality (positivity) follows from the data processing inequality for the relative entropy, so we only need to prove the equality. The proof only requires Lemma 14 and some algebraic manipulations. We have that

$$\frac{\mathrm{d}D(\rho_S(t)||\tau_S)}{\mathrm{d}t} = \lim_{h\to 0}\frac{D(\rho_S(t+h)||\tau_S) - D(\rho_S(t)||\tau_S)}{h} \quad (A.26)$$

$$= \lim_{h\to 0}\frac{\mathrm{Tr}[(\rho_S(t)+\mathcal{L}(\rho_S(t))h)(\log\{\rho_S(t)+\mathcal{L}(\rho_S(t))h\} - \log\tau_S)] - \mathrm{Tr}[\rho_S(t)(\log\rho_S(t)-\log\tau_S)]}{h} \quad (A.27)$$

$$= \lim_{h\to 0}\frac{1}{h}\Big[\mathrm{Tr}[(\rho_S(t)+\mathcal{L}(\rho_S(t))h)\{\log(\rho_S(t)) \quad (A.28)$$

$$+ h\int_0^1 \frac{1}{(1-x)\rho_S(t)+x\mathbb{I}}\mathcal{L}(\rho_S(t))\frac{1}{(1-x)\rho_S(t)+x\mathbb{I}}\mathrm{d}x\} - \log\tau_S)] - \mathrm{Tr}[\rho_S(t)(\log\rho_S(t)-\log\tau_S)]\Big]$$

$$= \mathrm{Tr}[\mathcal{L}(\rho_S(t))(\log\rho_S(t)-\log\tau_S)] + \mathrm{Tr}[\rho_S(t)\int_0^1 \frac{1}{(1-x)\rho_S(t)+x\mathbb{I}}\mathcal{L}(\rho_S(t))\frac{1}{(1-x)\rho_S(t)+x\mathbb{I}}\mathrm{d}x] \quad (A.29)$$

$$= \mathrm{Tr}[\mathcal{L}(\rho_S(t))(\log\rho_S(t)-\log\tau_S)] + \mathrm{Tr}[\rho_S(t)\mathcal{L}(\rho_S(t))\int_0^1\Big(\frac{1}{(1-x)\rho_S(t)+x\mathbb{I}}\Big)^2\mathrm{d}x]. \quad (A.30)$$

Where to go from the 2nd to the third line we used Lemma 14, and from the 4th to the 5th we use the ciclicity and linearity of the trace. Now note the following integral

$$\int_0^1\Big(\frac{1}{(1-x)p+x}\Big)^2\mathrm{d}x = \frac{1}{p}\ \ \forall p\neq 0. \quad (A.31)$$

This means that, on the support of $\rho_S(t)$,

$$\int_0^1\Big(\frac{1}{(1-x)\rho_S(t)+x\mathbb{I}}\Big)^2\mathrm{d}x = \frac{1}{\rho_S(t)}. \quad (A.32)$$

Note that outside the support of $\rho_S(t)$ this integral is not well defined. Given this, we can write

$$\frac{\mathrm{d}D(\rho_S(t)||\tau_S)}{\mathrm{d}t} = \mathrm{Tr}[\mathcal{L}(\rho_S(t))(\log\rho_S(t)-\log\tau_S)] + \mathrm{Tr}[\mathcal{L}(\rho_S(t))\Pi_{\rho_S(t)}], \quad (A.33)$$

where $\Pi_{\rho_S(t)}$ is the projector onto the support of $\rho_S(t)$. The Lindbladian is traceless $\mathrm{Tr}[\mathcal{L}(\rho_S(t))] = 0$ and hence second term of this Equation vanishes as long as $\mathrm{supp}(\mathcal{L}(\rho_S(t))) \subseteq \mathrm{supp}(\rho_S(t))$, which we can expect for most times. At instants in time when this is not the case and this term may give a finite contribution (that is, when the rank increases), the first term in Eq. (A.33) diverges logarithmically [165], and hence that finite contribution is negligible. □

A similar reasoning can be used to show that the instantaneous lower bound on entropy production rate that we can get from our main result in Eq. (4.79) is essentially trivial. In particular, we can show

**Lemma 15.** *The lower bound of Eq.* (4.79) *vanishes in the limit of infinitesimal time transformations. More precisely, we have that*

$$\lim_{h\to 0} \frac{D(\rho_S(t)||\rho_S(t+2h))}{h} = -2\,Tr[\mathcal{L}(\rho_S(t))\Pi_{\rho_S(t)}], \tag{A.34}$$

*where* $\Pi_{\rho_S(t)}$ *is the projector onto the support of* $\rho_S(t)$. *This vanishes as long as* $supp(\mathcal{L}(\rho_S(t))) \subseteq supp(\rho_S(t))$.

*Proof.* The proof is similar to the one for Theorem 26 above.

$$\lim_{h\to 0} \frac{D(\rho_S(t)||\rho_S(t+2h))}{h} = \lim_{h\to 0} \frac{1}{h}\mathrm{Tr}[\rho_S(t)(\log\rho_S(t) - \log(\rho_S(t) + 2h\mathcal{L}(\rho_S(t))))] \tag{A.35}$$

$$= \mathrm{Tr}[-2\rho_S(t)\int_0^1 \frac{1}{(1-x)\rho_S(t)+x\mathbb{I}}\mathcal{L}(\rho_S(t))\frac{1}{(1-x)\rho_S(t)+x\mathbb{I}}\mathrm{d}x\}] \tag{A.36}$$

$$= -2\mathrm{Tr}[\mathcal{L}(\rho_S(t))\Pi_{\rho_S(t)}], \tag{A.37}$$

where in the second line we applied Lemma 14, and in the third we used Eq. (A.32). □

Hence for infinitesimal times, the lower bound gives the same condition as the positivity condition in Eq. (A.25). It will be nonzero only when $\mathrm{supp}(\mathcal{L}(\rho_S(t))) \nsubseteq \mathrm{supp}(\rho_S(t))$, in which case the rate of entropy production diverges (at points in time when the rank of the system increases).

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