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The Properties of Thermodynamical Operations

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Abstract

The resource theory approach is a recently developed framework used in the study of thermodynamics for finite sized quantum systems. A simple way to describe how a quantum system evolves under energy-preserving unitaries while interacting with thermal reservoirs, has been formulated in the framework of thermal operations. Despite the conceptual simplicity of these operations, much is still unknown about their mathematical structures. In this work, we studied these mathematical structures, in an attempt to better understand how these operations, and some variants, describe quantum thermodynamics.

One of the interesting phenomena that occurs in quantum thermodynamics, is something that we call super-activation. In this phenomenon, we make multiple forbidden transitions possible by combining them together. This phenomenon could, for example, be used to extract more work from two systems, while it is impossible to extract any work from the individual systems. We found conditions for when this phenomenon can occur. As a result of this, we found that qubits with trivial Hamiltonians cannot super-activate each other. On the other hand, we found a way to construct infinitely many examples of super-activation.

We also investigated what happens if we combine multiples of the same forbidden transitions together. We found necessary conditions which each have to satisfy in order for this joint transition to be possible. In particular, these conditions show that this special case of super-activation can only occur in one direction.

Another topic that we studied in this work is smoothed Rényi divergences. In an attempt to give an operational meaning to these quantities, we studied two special states that allow us to clarify the relation between the smoothed Rényi divergences with the possibility of a transition. These special states are the steepest state and the flattest state. For a given state ρ, the steepest state is a state that is ϵ-close to ρ in terms of trace distance and can be transformed, in the presence of a thermal bath and while conserving the total energy, to any other state that is also ϵ-close to ρ. The flattest state is a state that is also ϵ-close to ρ in terms of trace distance, but all ϵ-close states of ρ can be transformed to it. We found a way to construct this steepest state for limited values of ϵ, and the flattest state for any ϵ.

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1 Introduction

Present-day technology is focusing a lot on reducing the size of systems, such as processors and cooling devices [8]. As these systems keep getting smaller, knowledge about thermodynamics on a small-scale level is becoming increasingly important. However, thermodynamics cannot properly be applied to these systems; it assumes that systems consist of infinitely many particles, which is no longer a good approximation for some extremely small systems.

A simple way to describe how a quantum system evolves under energy-preserving unitaries while interacting with thermal reservoirs, has been formulated in the framework of thermal operations. By allowing the use of ancillary states as catalysts in these processes, a more general set of thermodynamical operations is obtained, called catalytic thermal operations. Only recently, it was shown that in the quantum regime, the second law of thermodynamics takes a different form. Instead of just one law, a family of generalized second laws hold, with the original law being one instance of this infinite family of laws [2]. These laws govern the transitions that catalytic thermal operations can perform.

Despite the conceptual simplicity of these two types of thermodynamical operations, much is still unknown about their mathematical structures. In this work, we further investigate these operations and their properties, in order to better understand how they describe thermodynamics in the quantum regime. The main focus will be on super-activation. This is a phenomenon where we combine forbidden transitions, such that the combined transition is possible. The reason this phenomenon could be useful, is that in particular work could be super-activated. Even though we might be unable to draw more work from two individual systems, by combining them we could possibly draw more work from the joint system. This could make many processes, such as quantum computing, more efficient.

One of the goals of this project is to better understand this phenomenon. We will search for restrictions on when we cannot super-activate systems, and look for ways to construct examples. We will also investigate a special case of super-activation that we call self-activation. Here, instead of combining two arbitrary transitions, we will combine multiple of the same transition.

Another question that is of interest, arises from the fact that many of the relevant quantities that are important in quantum thermodynamics find their origin in information theory [7]. Examples of these quantities are the Rényi entropy and Rényi divergences. In particular, smoothed Rényi divergences bring up questions. These are defined in such a way that it is unclear what their physical meaning is, despite their importance in quantum thermodynamics. We will try to find out more about these divergences. Furthermore, we will investigate the steepest and flattest states, that turn out to be relevant when looking at these divergences.

This thesis consists of five chapters. In chapter 2 we discuss the background knowledge that this work relies on. We first discuss the basics of quantum mechanics, and after that we define the thermodynamical operations of interest.

Chapter 3 includes the results regarding super-activation, which is a phenomenon where combining forbidden state transitions can make both transitions possible. In the first section of this chapter we focus on the case where the Hamiltonians are fully degenerate. We show that qubits cannot super-activate each other, and we give a way to construct examples of the phenomenon. We also find necessary conditions for self-activation, which is the special case of super-activation where multiples of the same transition are combined. In the second section of chapter 3, we turn to more general Hamiltonians. In chapter 4, we investigate the smoothed Rényi divergences, as well as steepest and flattest states. We provide a way to construct these states, and give conditions for when the steepest state exists. We also show that the flattest state always exists.

Finally, in chapter 5 we give a summary of our results, as well as some suggestions for further research.

2 Preliminaries

In this chapter, we discuss the background knowledge that is needed to understand the used methods and the results. First, we explain some terminology and notation for quantum mechanical systems. This section is mainly based on [9,10]. Secondly, we discuss different types of thermodynamical operations and their properties. Lastly we give some criteria that govern state transitions. These criteria will be used extensively in most of the results.

2.1 Quantum systems

2.1.1 Pure states

Quantum mechanics revolve around the properties of tiny particles. These properties define the state of a quantum system. An example of such a property is the spin of an electron. To describe the state of these particles, we use vectors in Hilbert spaces. We generally denote these quantum states by $|\psi\rangle$, which is called the bra-ket notation. The complex conjugate transpose of $|\psi\rangle$ is given by $|\psi\rangle^\dagger = \langle\psi|$. Sometimes this is also written as $|\psi\rangle^*$.

Quantum states can be either pure or mixed. A quantum state is called pure when one can say with certainty that the quantum system is in that particular state. Because these states are solutions of the Schrödinger equation, we can add them together to form superpositions of states, which are also solutions of the Schrödinger equation. These superpositions of states are pure states as well. For qubits, which are two dimensional systems, superposition takes the form $|\psi\rangle = c_1 |0\rangle + c_2 |1\rangle$, where $|c_1|^2 + |c_2|^2 = 1$.

Before moving on to mixed states, we will first explain the basics of Hamiltonians.

2.1.2 Hamiltonians

The time-independent Schrödinger equation is given by

$$\hat{H} |\psi\rangle = E |\psi\rangle . \tag{1}$$

Here, $\hat{H}$ is the Hamiltonian operator, which corresponds with the total energy of a quantum state. Hamiltonians are Hermitian linear operators on states. They determine how states evolve with time. This evolution is given by the unitary operator $U = e^{-i\hat{H}t}$, such that

$$|\psi\rangle' = U |\psi\rangle . \tag{2}$$

Unitary operators preserve the energy of the system, and satisfy $U^{-1} = U^{\dagger}$.

Hamiltonians determine the energy eigenstates, and how much energy these would have: these eigenstates are the eigenvectors of the Hamiltonian, and the corresponding energy levels are the eigenvalues. Because Hamiltonians are Hermitian operators, their eigenvalues are always real. We will give a brief example to illustrate these operators.

Example 2.1. Consider the d-dimensional system with the Hamiltonian given by

$$\hat{H} = I_d, \tag{3}$$

where I_d is the d-dimensional identity matrix. Such a Hamiltonian is called a trivial or fully-degenerate Hamiltonian. Then, the Schrödinger equation becomes

$$\hat{H} \left|\psi\right\rangle = cI_d \left|\psi\right\rangle = c \left|\psi\right\rangle = E \left|\psi\right\rangle. \tag{4}$$

The only solution of this equation, is $E = c$ for any $\left|\psi\right\rangle$. Thus, all states of this system have the same amount of energy.

This has many consequences. First of all, any unitary would commute with such a Hamiltonian. This means that any unitary operator would be energy preserving for such a system. Another consequence is that one of the criteria that govern state transitions reduces to a much simpler variant for trivial Hamiltonians. We will discuss this later. The latter is the main reason we will start out by examining systems with trivial Hamiltonians.

2.1.3 Mixed states

As we stated before, not all quantum states are pure states. Often, rather than being certain about the state of a quantum system, the state is a probabilistic mixture of pure states. This simply means that for every pure state, we have a probability to find the system in this pure state.

A special case of a mixed state is the thermal state. This state is also called the maximally mixed state, or the Gibbs state. The probability that the thermal state is found in an eigenstate with energy E_i is given by

$$p_i = \frac{e^{-\beta E_i}}{Z}. \tag{5}$$

Here, $\beta = \frac{1}{T}$ is the inverse temperature and Z is the partition function, defined as

$$Z = \sum_{i=1}^{d} e^{-\beta E_i}. \tag{6}$$

2.1.4 Density matrices

Clearly, mixed states cannot be expressed with state vectors like pure states can. Instead, we use density matrices to express states. Density matrices can be used to express both pure and mixed states, which makes them very convenient. The density matrix of a quantum state, pure or mixed, is given by

$$\rho = \sum_i p_i \left|\psi_i\right\rangle \left\langle\psi_i\right|, \tag{7}$$

where p_i is the probability that the quantum system is found in the state $|\psi_i\rangle$. When $|\psi\rangle_i$ are orthogonal, these probabilities are the eigenvalues of the density matrix. From this definition, it becomes clear that density matrices are Hermitian. As a result, the eigenvalues of density matrices are real. Furthermore, the eigenvalues are non-negative and sum up to 1. This means that the eigenvalues of a density matrix form a discrete normalized probability distribution.

The eigenvalues of a density matrix play an important role when calculating the trace of the matrix. The trace of a square matrix is defined as

$$\operatorname{tr}(\rho) = \sum_i \rho_{ii}, \tag{8}$$

where ρ_{ii} denotes the ii-th entry of ρ. The trace of a matrix is invariant under basis transformation. Since density matrices are hermitian, we can diagonalize them, which results in the eigenvalues appearing on the diagonal. As a direct result, the trace of a density matrix is is also equal to the sum of the eigenvalues. This yields

$$\operatorname{tr}(\rho) = 1. \tag{9}$$

2.2 Joint systems

So far we have only considered single systems. However, often we are interested what happens if we combine multiple systems. Therefore, having a way to describe the state of multiple systems at the same time would be very useful.

2.2.1 Tensor products

Let $|\psi_A\rangle$ and $|\psi_B\rangle$ be states of two different d_A- and d_B-dimensional systems. Then, if there is no interaction between the systems, the joint state can be expressed as

$$\left|\psi_{AB}\right\rangle = \left|\psi_A\right\rangle \otimes \left|\psi_B\right\rangle. \tag{10}$$

Here, $\otimes$ is the tensor product, which acts on two matrices A with entries a_{ij} and B with entries b_{ij}, such that

$$A \otimes B = \begin{bmatrix} a_{11}B & a_{12}B & \dots & a_{1d_A}B \\ a_{21}B & a_{22}B & & \\ \vdots & & \ddots & \\ a_{d_A1}B & & & a_{d_Ad_A}B \end{bmatrix}. \tag{11}$$

Tensor products can also be used to combine many of the same states together. This leads to the usage of the tensor power, which is defined as

$$A^{\otimes n} = A \otimes \ldots \otimes A. \tag{12}$$

Notice that tensor products quickly inflate the dimension of the density matrices; combining even a few systems together can result in huge dimensions.

2.2.2 Partial trace

The trace operator can be generalized to the partial trace. For a bipartite state ρ_{AB}, and an orthonormal basis of $\mathcal{H}_B$ given by $\{|l\rangle_B\}$, the partial trace over B is defined as

$$\mathrm{tr}_B(\rho_{AB}) = \sum_l \left(I_A \otimes \langle l|_B\right) \rho_{AB} \left(I_A \otimes |l\rangle_B\right). \tag{13}$$

For a product state $\rho_{AB} = \rho_A \otimes \rho_B$, this yields

$$\mathrm{tr}_B(\rho_{AB}) = \rho_A. \tag{14}$$

We call ρ_A the reduced state on A.

2.2.3 Joint Hamiltonians

For the joint state as described above, we would also like to define the joint Hamiltonian. Let $\hat{H}_A$ be the Hamiltonian of system A, and $\hat{H}_B$ the Hamiltonian of system B. Let $\left\{|\psi_i^A\rangle\right\}$ be the eigenstates of $\hat{H}_A$, with corresponding eigenvalues $\left\{E_i^A\right\}$, and let $\left\{|\psi_i^B\rangle\right\}$ be the eigenstates of $\hat{H}_B$, with corresponding eigenvalues $\left\{E_i^B\right\}$. As we mentioned earlier, we assume that there is no interaction between the systems. In other words, the Hamiltonian of system A does not act on system B, and neither does the Hamiltonian of system B act on system A. The joint Hamiltonian becomes

$$\hat{H}_{AB} = \hat{H}_A \otimes I_{d_B} + I_{d_A} \otimes \hat{H}_B. \tag{15}$$

We can verify that the eigenstates and corresponding energy levels of the individual systems remain unchanged, such that $|\psi_{ij}^{AB}\rangle = |\psi_i^A\rangle \otimes |\psi_j^B\rangle$ is an eigenstate of the joint Hamiltonian. We have that

$$
\begin{aligned}
\hat{H}_{AB} \left|\psi_{ij}^{AB}\right\rangle &= \left(\hat{H}_A \otimes I_{d_B} + I_{d_A} \otimes \hat{H}_B\right) \left(\left|\psi_i^A\right\rangle \otimes \left|\psi_j^B\right\rangle\right) && (16)\\
&= \left(E_i^A \left|\psi_i^A\right\rangle\right) \otimes \left|\psi_j^B\right\rangle + \left|\psi_i^A\right\rangle \otimes \left(E_j^B \left|\psi_j^B\right\rangle\right) && (17)\\
&= \left(E_i^A + E_j^B\right) \left|\psi_i^A\right\rangle \otimes \left|\psi_j^B\right\rangle && (18)\\
&= E_{ij} \left|\psi_{ij}^{AB}\right\rangle, && (19)
\end{aligned}
$$

where $E_{ij} = E_i^A + E_j^B$ is the energy of this eigenstate. We will denote this joint Hamiltonian as

$$\hat{H}_{AB} = \hat{H}_A + \hat{H}_B. \tag{20}$$

2.3 Thermodynamical operations

2.3.1 Quantum channels

Since we are interested in the thermodynamical interactions between a system and its surroundings, it is not just the quantum states that we are interested in. We are especially interested in the state transitions that occur as the system interchanges information with the thermal bath.

In quantum mechanics, state transitions can be described by quantum channels. Quantum channels are completely positive trace-preserving maps, that map density matrices onto density matrices. The time evolution of a state that we gave earlier, can also be expressed as a quantum channel, such that

$$\rho' = U\rho U^{\dagger}. \tag{21}$$

The reason that quantum channels must be trace preserving, is that when we apply a quantum channel to a density matrix, the output should still be a density matrix. Since all density matrices have trace 1, both the input and the output of the quantum channel have the same trace. Another important restriction to the linear maps that are allowed in quantum channels, is that the maps need to be completely positive. This ensures that even when dealing with entangled states, the output of the channel is a physical state.

2.3.2 Thermal operations

The most basic type of quantum channel we will be looking at is the thermal operation. Thermal operations describe the thermodynamical interactions between a quantum system and an equilibrated environment. They are defined as

$$\mathcal{E}_{TO}(\rho) = \mathrm{tr}_B \left[U_{SB} \left(\rho \otimes \tau_B\right) U_{SB}^{\dagger}\right]. \tag{22}$$

Here, τ_S is the thermal state, and U_{SB} is a unitary operation. Since we are looking at energy preserving operations, the quantum channel is restricted such that the unitary commutes with the joint Hamiltonian. This can be expressed as

$$[U_{SB}, \hat{H}_S + \hat{H}_B] = 0. \tag{23}$$

This restriction will ensure that no energy will be added or removed from the joint system by the thermal operation. This is why the presence of the thermal bath is so important. Without it, the energy of the system could never change.

Despite the conceptual simplicity of this type of quantum channel, much is still unknown about the properties thereof. We will give a quick overview of what is known right now.

First of all, it is known that the set of thermal operations forms a convex set. This means that any convex combination of two arbitrary thermal operations, is again a thermal operation. This gives us that

$$\alpha\mathcal{E}^1_{TO}(\rho) + \beta\mathcal{E}^2_{TO}(\rho) = \mathcal{E}^3_{TO}(\rho). \tag{24}$$

Another property that thermal operations have, is that they cannot generate coherent superpositions starting from an energy eigenstate.

Finally, thermal operations preserve the thermal state if the system has the same temperature as the bath. This means that for all thermal operations,

$$\mathcal{E}_{TO}(\tau_S) = \tau_S. \tag{25}$$

The conditions that determine whether or not state transitions are possible, are known as thermo-majorization, which we will discuss in section 2.4.1.

2.3.3 Catalytic thermal operations

Catalytic thermal operations are very similar to thermal operations. The difference between the two is that with catalytic thermal operations we may use a catalyst, which is simply an additional finite-dimensional quantum system, that is returned exactly. These operations are defined as

$$\mathcal{E}_{CTO}(\rho) = \mathrm{tr}_{BC}\left[U_{SBC}\left(\rho \otimes \omega_C \otimes \tau_B\right) U^\dagger_{SBC}\right]. \tag{26}$$

Here, τ_S is again the thermal state, and U_{SBC} is a unitary operation. Since we are still looking at energy preserving operations, the unitary U_{SBC} has to commute with the joint Hamiltonian, just as for thermal operations. We have that

$$[U_{SBC}, \hat{H}_S + \hat{H}_B + \hat{H}_C] = 0. \tag{27}$$

Furthermore, the catalyst has to be returned exactly, and has to be uncorrelated with the system, such that

$$\mathrm{tr}_B \left[U_{SBC} \left(\rho \otimes \omega_C \otimes \tau_B \right) U^\dagger_{SBC} \right] = \mathcal{E}_{CTO}(\rho) \otimes \omega_C. \tag{28}$$

We will list some of the properties of catalytic thermal operations that are currently known.

First of all, the set of catalytic thermal operations includes the set of thermal operations. That this is the case, can be seen by looking at an arbitrary thermal operation. We can add a catalyst and return it, while leaving it untouched by the unitary. This defines a catalytic thermal operation that performs the same transition as the thermal operation.

Just like thermal operations, they preserve the Gibbs state, such that

$$\mathcal{E}_{CTO}(\tau_S) = \tau_S. \tag{29}$$

Both sets are not the same, however. The presence of a catalyst enables us to perform transitions that we would not be able to perform without it.

As we stated in the previous section, the set of thermal operations is convex. It was not clear if the same was true for catalytic thermal operations. Similar to how it was proved that the set of thermal operations is convex in [6], we proved that the set of catalytic thermal operations is convex. We give the proof below.

Theorem 1. *The set of catalytic thermal operations is convex.*

Proof. Let $\mathcal{E}_1$ and $\mathcal{E}_2$ be catalytic thermal maps acting on a system ρ_S, such that

$$\mathcal{E}_1(\rho_S) = tr_{C_1B_1} \left[U_{SB_1}(\rho_S \otimes \omega_{C_1} \otimes \tau_{B_1}) U^\dagger_{SB_1} \right] \tag{30}$$

$$\mathcal{E}_2(\rho_S) = tr_{C_2B_2} \left[U_{SB_2}(\rho_S \otimes \omega_{C_2} \otimes \tau_{B_2}) U^\dagger_{SB_2} \right]. \tag{31}$$

The thermal states are given by

$$\tau_{B_1} = \frac{e^{-\beta H_{B_1}}}{Z_1}, \tau_{B_2} = \frac{e^{-\beta H_{B_2}}}{Z_2}. \tag{32}$$

Notice that they have the same temperature. First, we introduce a d-dimensional ancillary bath state τ_A with Hamiltonian $H_A = I_d$. Define the controlled unitary

$$U := \Pi_1 \otimes U_{SB_1} + \Pi_2 \otimes U_{SB_2}. \tag{33}$$

Where Π_1 and Π_2 are rank k and rank $d-k$ projectors onto the degenerate bath system of the ancilla A respectively, and $\Pi_1 + \Pi_2 = I_d$. We check if this operator commutes with the shared Hamiltonian:

$$\begin{aligned}
[U, H] &= [\sum_{i=1}^{2} \Pi_i \otimes U_{SB_i}, H_S + H_A + \sum_{j=1}^{2} H_{B_j} + H_{C_j}] && (34)\\
&= \sum_{i=1}^{2} \left([\Pi_i \otimes U_{SB_i}, H_S + H_A] + \sum_{j=1}^{2} \Pi_i \otimes [U_{SB_i}, H_{B_j} + H_{C_j}] \right). && (35)
\end{aligned}$$

Note that U_{SB_i} leaves τ_{B_j} and ω_{C_j} unchanged if $i \neq j$. In other words, U_{SB_i} commutes with H_{B_j} and H_{C_j}. Also notice that everything commutes with H_A, which means that H_A can be ignored. We have that

$$\begin{aligned}
[U, H] &= \sum_{i=1}^{2} (\Pi_i \otimes [U_{SB_i}, H_S] + \Pi_i \otimes [U_{SB_i}, H_{B_i} + H_{C_i}]) && (36)\\
&= \sum_{i=1}^{2} \Pi_i \otimes [U_{SB_i}, H_S + H_{B_i} + H_{C_i}]. && (37)
\end{aligned}$$

By definition, u_{SB_i} commutes with $H_S + H_{B_i} + H_{C_i}$. This yields

$$[U, H] = 0. \tag{38}$$

Thus, U commutes with the total Hamiltonian. Next, we compute the state of ρ_S after applying U to it. We have that

$$\begin{aligned}
\rho'_S &= tr_{AC_1C_2B_1B_2}\left[U(\rho_S \otimes \omega_{C_1} \otimes \omega_{C_2} \otimes \tau_A \otimes \tau_{B_1} \otimes \tau_{B_2})U^\dagger\right] && (39)\\
&= \frac{1}{d} tr_{AC_1C_2B_1B_2}\left[U(\rho_S \otimes \omega_{C_1} \otimes \omega_{C_2} \otimes \mathbb{I}_d \otimes \tau_{B_1} \otimes \tau_{B_2})U^\dagger\right] && (40)\\
&= \frac{1}{d} \sum_{i=1}^{2} \sum_{j=1}^{2} tr_{AC_1C_2B_1B_2}[\Pi_i \otimes U_{SB_i}(\rho_S \otimes \omega_{C_1} \otimes \omega_{C_2} \otimes \mathbb{I}_d \otimes \tau_{B_1} \otimes \tau_{B_2})\Pi_j \otimes U^\dagger_{SB_j}] && (41)\\
&= \frac{1}{d} \sum_{i=1}^{2} \sum_{j=1}^{2} tr_A[\Pi_i \Pi_j] tr_{C_1C_2B_1B_2}[U_{SB_i}(\rho_S \otimes \omega_{C_1} \otimes \omega_{C_2} \\
&\quad \otimes \tau_{B_1} \otimes \tau_{B_2})U^\dagger_{SB_j}]. && (42)
\end{aligned}$$

Using the fact that Π_1 and Π_2 are projectors onto the degenerate bath system, such that $\Pi_1 + \Pi_2 = I$, we can simplify this expression. Namely, we have that the ii-th element of $\Pi_1\Pi_2$ equals 0 for all i. Therefore, we have that $tr_A[\Pi_i\Pi_j] = 0$ if $i \neq j$. Furthermore, we have that $tr_A[\Pi_i\Pi_i] = tr_A[\Pi_i]$. Thus, we have that

$$\begin{aligned}
\rho'_S &= \frac{1}{d}\sum_{i=1}^{2} tr_A[\Pi_i] tr_{C_1C_2B_1B_2}[U_{SB_i}(\rho_S \otimes \omega_{C_1} \otimes \omega_{C_2} \otimes \tau_{B_1} \otimes \tau_{B_2})U^\dagger_{SB_i}] && (43)\\
&= \frac{1}{d}\sum_{i=1}^{2} tr_A[\Pi_i] tr_{C_iB_i}[U_{SB_i}(\rho_S \otimes \omega_{C_i} \otimes \tau_{B_i})U^\dagger_{SB_i}] && (44)\\
&= \frac{k}{d}\mathcal{E}_1(\rho_S) + \left(1 - \frac{k}{d}\right)\mathcal{E}_2(\rho_S). && (45)
\end{aligned}$$

Here, we used that Π_1 is a rank k projector, and Π_2 is a rank $d-k$ projector onto the degenerate bath system. We only have to verify that the catalyst remains unchanged. We determine the final state of $\omega_{C_1} \otimes \omega_{C_2}$, which is given by

$$\begin{aligned}
\omega'_1 \otimes \omega'_2 &= tr_{ASB_1B_2}\left[U(\rho_S \otimes \omega_{C_1} \otimes \omega_{C_2} \otimes \tau_A \otimes \tau_{B_1} \otimes \tau_{B_2})U^\dagger\right] && (46)\\
&= \frac{1}{d} tr_{ASB_1B_2}\left[U(\rho_S \otimes \omega_{C_1} \otimes \omega_{C_2} \otimes \mathbb{I}_d \otimes \tau_{B_1} \otimes \tau_{B_2})U^\dagger\right] && (47)\\
&= \frac{1}{d}\sum_{i=1}^{2}\sum_{j=1}^{2} tr_{ASB_1B_2}[\Pi_i \otimes U_{SB_i}(\rho_S \otimes \omega_{C_1} \otimes \omega_{C_2} \otimes \mathbb{I}_d \otimes \tau_{B_1} \otimes \tau_{B_2})\Pi_j \otimes U^\dagger_{SB_j}] && (48)\\
&= \frac{1}{d}\sum_{i=1}^{2}\sum_{j=1}^{2} tr_A[\Pi_i\Pi_j] tr_{SB_1B_2}[U_{SB_i}(\rho_S \otimes \omega_{C_1} \otimes \omega_{C_2} \otimes \tau_{B_1} \otimes \tau_{B_2})U^\dagger_{SB_j}] && (49)\\
&= \frac{1}{d}\sum_{i=1}^{2} tr(\Pi_i) tr_{SB_i}\left[U_i(\rho_S \otimes \omega_{C_1} \otimes \omega_{C_2} \otimes \tau_{B_i})U_i^\dagger\right] && (50)\\
&= \frac{k}{d}(\omega_{C_1} \otimes \omega_{C_2}) + \left(1 - \frac{k}{d}\right)(\omega_{C_1} \otimes \omega_{C_2}) && (51)\\
&= \omega_{C_1} \otimes \omega_{C_2}. && (52)
\end{aligned}$$

Thus, the catalyst is returned to its original state. Therefore $(U, \tau_A \otimes \tau_1 \otimes \tau_2, \omega_1 \otimes \omega_2)$ defines a catalytic thermal map equivalent to any rational convex combination of $(U_{SB_1}, \tau_1, \omega_1)$ and $(U_{SB_2}, \tau_2, \omega_2)$. Irrational combinations are approached with arbitrary accuracy. Thus, the set of catalytic thermal maps is convex. □

2.3.4 Gibbs-preserving maps

Gibbs-preserving maps form an even more general class of thermodynamical operations. A quantum channel is called Gibbs-preserving simply if it preserves the Gibbs state, such that

$$\mathcal{E}_{GP}(\tau_S) = \tau_S. \tag{53}$$

From the definition it becomes clear that this set includes all catalytic thermal operations, and therefore all thermal operations as well, since they too preserve the Gibbs state. However, this set is bigger than the previous sets of thermodynamical operations. Namely, Gibbs-preserving maps can outperform thermal operations; for example, Gibbs-preserving maps can generate coherent superpositions starting from an energy eigenstate [5].

Another property that Gibbs-preserving maps satisfy, is that they form a convex set. This can be seen by considering any convex combination of Gibbs-preserving maps: this combination would also preserve the Gibbs state.

Because Gibbs-preserving maps can do anything thermal operations or catalytic thermal operations can do, and more, they may seem like the most interesting set of quantum channels to study. It is, however, unclear if it is possible to actually create all Gibbs-preserving maps, unlike thermal and catalytic thermal operations. Being able to realize these quantum channels is of great importance. Therefore, we will mainly focus on thermal operations and catalytic thermal operations in this work.

2.4 Transition conditions

2.4.1 Thermo-majorization

One way to find out if a certain transition $\rho \to \sigma$ is possible, would be to explicitly find the corresponding thermal operations, though this can be very difficult. Fortunately, there is a very powerful criterion that tells us whether or not a transition between two states is possible by thermal operations. This criterion is called thermo-majorization. Thermo-majorization compares two curves that correspond to the states in question. A thermal operation can perform the transition $\rho \to \sigma$ if and only if the thermo-majorization curve of ρ lies above the thermo-majorization curve of σ [1].

The thermo-majorization curve of a state ρ that is block diagonal in its energy eigenbasis is constructed as follows. Let the eigenvalues of ρ be given by $\{p_i\}$, and let the corresponding energy levels be given by $\{E_i\}$. We start by putting these eigenvalues in a specific order called the β-order, which we define below.

Definition 2.1. Let ρ be a state that is block diagonal in its energy eigenbasis, with eigenvalues $\{p_i\}$ and corresponding energy levels $\{E_i\}$. The eigenvalues of ρ are said to be β-ordered if $p_1 e^{\beta E_1} \geq p_2 e^{\beta E_2} \geq \dots$, where $\beta = \frac{1}{T}$.

The thermo-majorization curve of ρ is then given by the straight lines connecting the points $\left\{\left(\sum_{i=1}^{k} e^{-\beta E_i}, \sum_{i=1}^{k} p_i\right)\right\}$. We will give an example of thermo-majorization for different states.

Example 2.2. Let ρ, σ and τ be 4-dimensional quantum systems. Let the eigenvalues of ρ, σ and τ be given by respectively $\{0.6, 0.3, 0.08, 0.02\}$, $\{0.7, 0.15, 0.1, 0.05\}$ and $\{0.1558, 0.2598, 0.1948, 0.3896\}$. For the sake of simplicity, we will define the values of $\{e^{\beta E_i}\}$ rather than defining the energy levels themselves. Let $\{e^{\beta E_i}\}$ of ρ, σ and τ be given by $\{5, 3, 4, 2\}$. Notice that the eigenvalues of all three states are β-ordered. We give the thermo-majorization diagram of all three states in figure 1.

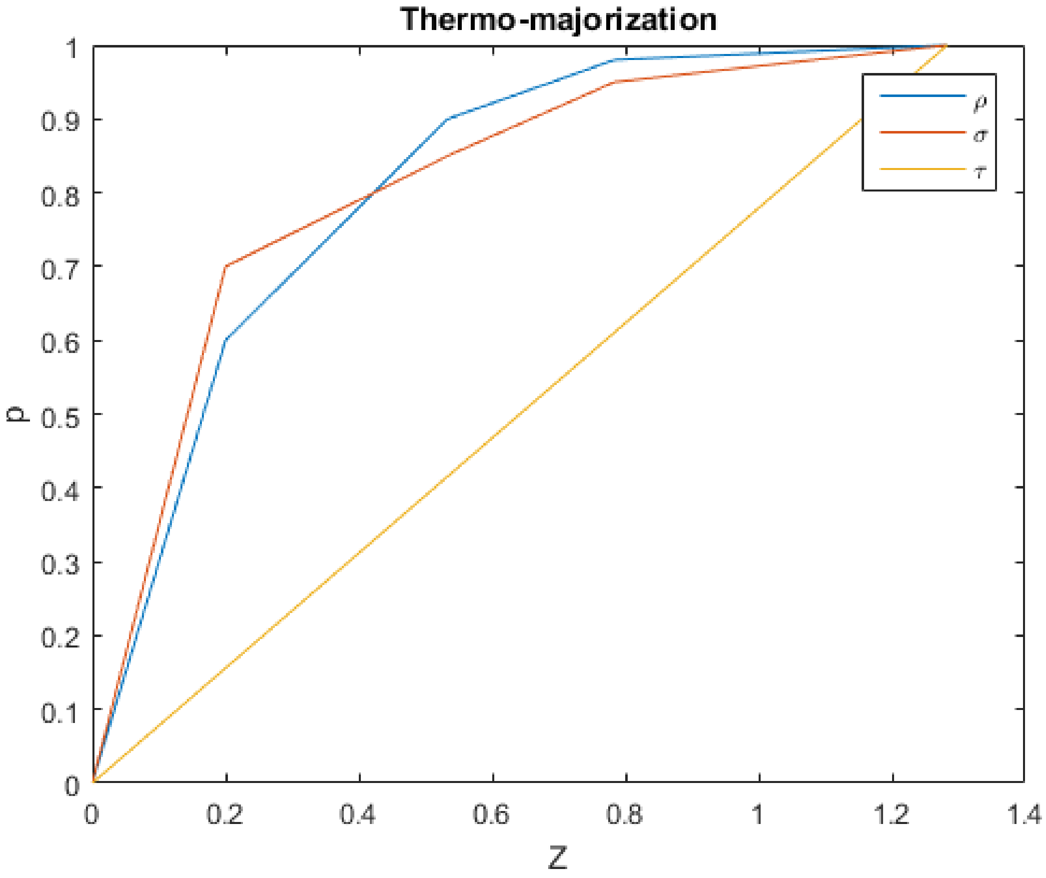

Figure 1: The majorization diagram of three different states, ρ, σ and the thermal state τ. Here, $Z = \sum_{i=1}^{d} e^{-\beta E_i}$ denotes the partition function. The points $\left\{\left(\sum_{i=1}^{k} e^{-\beta E_i}, \sum_{i=1}^{k} p_i\right)\right\}$ have been marked for each state. Notice that the curves for ρ and σ intersect, meaning that these states cannot be transformed to each other. Also, notice that both ρ and σ can be transformed to the thermal state.

The states ρ and σ are said to be incomparable; neither of the two can be transformed to the other.

Because the eigenvalues of the states are β-ordered before the curve is constructed, all thermo-majorization curves are concave. This β-order does not have to be the same for different states of the same system, like it was in the example. This can make it much more difficult to compare the curves of two states, or to construct states with a specific curve. Fortunately, when the Hamiltonians are trivial, this problem vanishes. We will explain this more in depth.

Consider the d-dimensional systems ρ and σ with trivial Hamiltonians. As we showed earlier, because the Hamiltonian is trivial, all energy levels have the same amount of energy. Let p_i and q_i be the β-ordered eigenvalues of ρ and σ respectively. Because the Hamiltonian is trivial, we have that $e^{-\beta E_i} = c$, with c a constant. This means that the β-order reduces to $p_1 \geq p_2 \geq \ldots \geq p_d$. We will proceed to construct the thermo-majorization curves for both states.

For ρ, the thermo-majorization curve is therefore given by the set of points $\left\{\left(\sum_{i=1}^{k} c, \sum_{i=1}^{k} p_i\right)\right\}$, and the thermo-majorization curve of σ is given by the set of points $\left\{\left(\sum_{j=1}^{k} c, \sum_{j=1}^{k} q_j\right)\right\}$.

In order to find out if the transition is possible, we need to compare the height of these two diagrams. Fortunately, because the Hamiltonian is trivial, the horizontal position of the points of both diagrams line up perfectly, and thus it is sufficient to check that at every vertex of the curves, ρ lies above σ. We only have to compare $\sum_{i=1}^{k} p_i$ and $\sum_{i=1}^{k} q_i$, for all $1 \leq k \leq d$. If for each of these k, we have that $\sum_{i=1}^{k} p_i \geq \sum_{i=1}^{k} q_i$, the transition is possible. In addition, because the states are normalized we have that $\sum_{i=1}^{d} p_i = \sum_{i=1}^{d} q_i$, this means that ρ majorizes σ. We denote this by $\rho \succ \sigma$.

When comparing the thermo-majorization curves of states, it is possible that neither $\rho \to \sigma$ nor $\sigma \to \rho$. In this case, we say that the states are incomparable. Incomparability will be an important quality, as we will explain in the results.

As we stated before, catalytic thermal operations can perform more transitions than thermal operations. The reason for this, is that catalysts affect the thermo-majorization curves. Clearly, thermo-majorization cannot be used to obtain information about catalytic thermal operations, other than the possibility of a transition with a certain catalyst. To find out if catalytic thermal operations can perform a transition, we need different tools.

2.4.2 Rényi entropies and divergences

Fortunately, a similar tool exists to find out if catalytic thermal operations can perform certain transitions. In information theory, two very important quantities are the Rényi entropies and Rényi divergences, and as it turns out, these quantities are important in quantum thermodynamics as well.

In the case that the Hamiltonians are trivial, a transition $\rho \to \sigma$ is possible if and only if for $\alpha \in \mathbb{R}$ [2],

$$H_\alpha(\rho) \leq H_\alpha(\sigma) \tag{54}$$

Here, H_α is the Rényi entropy, which is defined as

$$H_\alpha(\rho) = \frac{\operatorname{sgn}(\alpha)}{1-\alpha} \log \sum_i p_i^\alpha. \tag{55}$$

For states with nontrivial Hamiltonians that are block diagonal in the energy eigenbasis, we have to compare the Rényi divergences instead. A transition is possible if and only if $\alpha \in \mathbb{R}$,

$$D_\alpha(\rho||\tau) \geq D_\alpha(\sigma||\tau). \tag{56}$$

Here, the Rényi divergences are defined as

$$D_\alpha(\rho||\tau) = \frac{\operatorname{sgn}(\alpha)}{\alpha-1} \log \sum_i p_i^\alpha q_i^{1-\alpha}. \tag{57}$$

Unfortunately, for states that are not block diagonal, these conditions are only necessary, but insufficient. In this work, we will not consider states like these.

2.4.3 Super-activation

As we mentioned before, a transition that is impossible to achieve by thermal operations, may not be impossible if we add a catalyst to the system that is returned exactly. This leads to the question if other resources, that are by themselves not useful, could be added to make a transition possible. As it turns out, sometimes we can combine multiple forbidden transitions to make them possible. This is what we call super-activation. It can be expressed as

$$\rho_1 \otimes \rho_2 \to \sigma_1 \otimes \sigma_2, \tag{58}$$

while $\rho_1 \not\to \sigma_1$ and $\rho_2 \not\to \sigma_2$. Clearly, super-activation can be very useful; it allows us to potentially extract more work from two systems, that we cannot extract work from individually. In [3,4] they show that a transition $\rho \to \sigma$ can be superactivated if

$H(\rho) > H(\sigma)$, but the condition might not be necessary. Apart from examples, much is still unknown about the phenomenon, however.

2.4.4 Self-activation

Self-activation is a special case of super-activation, where we combine multiple of the same forbidden transitions in order to make them possible. This can be expressed as

$$\rho^{\otimes n} \to \sigma^{\otimes n}, \tag{59}$$

while ensuring that $\rho \not\to \sigma$. Notice that when catalysts are allowed, self-activation cannot happen. Due to the additive nature of the Rényi divergences, adding multiple copies of the same state together only multiplies the divergences by n, and thus this will never make the transition possible. This means that transitions that can be self-activated, can also be made possible by adding a catalyst.

2.4.5 Smoothing

Sometimes, rather than comparing two states we would like to say something about transitions of 'close' states. This leads to the use of the smoothed Rényi divergences. For $\epsilon > 0$, the smoothed Rényi divergences are defined as

$$D_\alpha^\epsilon(\rho||\tau) = \begin{cases} \min_{\tilde{\rho}} D_\alpha(\tilde{\rho}||\tau) & \text{if } \alpha < 0 \\ \max_{\tilde{\rho}} D_\alpha(\tilde{\rho}||\tau) & \text{if } 0 \leq \alpha \leq 1 \\ \min_{\tilde{\rho}} D_\alpha(\tilde{\rho}||\tau) & \text{if } \alpha > 1, \end{cases} \tag{60}$$

where optimization occurs over all states $\tilde{\rho}$ within the an ϵ-ball around ρ. These states satisfy

$$\tilde{\rho} : \frac{1}{2}\mathrm{Tr}\left[\sqrt{(\rho - \tilde{\rho})^\dagger(\rho - \tilde{\rho})}\right] \leq \epsilon. \tag{61}$$

For states that are diagonal in the same basis, this becomes

$$\tilde{\rho} : \frac{1}{2}\sum_i |p_i - \tilde{p}_i| \leq \epsilon. \tag{62}$$

Because the smooth Rényi divergences are defined differently for different regions, they do not, as a whole, correspond to the Rényi divergence of a single state. This removes any physical meaning of the quantity; it seems to be merely a tool. In this work, we investigate this physical meaning.

3 Super-activation

In this chapter, we will give all the results that are related to super-activation. In section 3.1 we analyze super-activation with trivial Hamiltonians. First, we show that qubits with trivial Hamiltonians cannot super-activate each other. Then, we show that we can always combine possible transitions, which will allow us to construct examples of super-activation. Lastly, we give necessary conditions for self-activation, as well as some consequences.

In section 3.2 we turn to nontrivial Hamiltonians. We give several examples that show that some of the theorems for the trivial case cease to hold for nontrivial Hamiltonians. These examples also hint at other theorems that we think can be extended for the nontrivial case.

3.1 Trivial Hamiltonians

In this section, we will give all the results that are related to super-activation with trivial Hamiltonians. Recall that a transition is super-activated if $\rho_1 \otimes \rho_2 \to \sigma_1 \otimes \sigma_2$, while at the same time $\rho_1 \not\to \sigma_1$, and $\rho_2 \not\to \sigma_2$.

We start by analyzing the simplest cases; as we showed in chapter 2, when looking at systems with trivial Hamiltonians, we only have to check majorization, rather than thermo-majorization, which makes things much easier.

3.1.1 2-dimensional systems

We will first analyze super-activation in 2-dimensional systems. For higher dimensional systems, see sections 3.1.2-3.1.4. To determine if the 2-dimensional system ρ, with eigenvalues p_i, majorizes the 2-dimensional system σ, with eigenvalues q_i, we have to check that for $k = 1, 2$,

$$\sum_{i=1}^{k} p_i \geq \sum_{i=1}^{k} q_i. \tag{63}$$

However, for $k = 2$ this is always true, because the eigenvalues are normalized. Thus, majorization reduces to the comparison of p_1 and q_1. $\rho \succ \sigma$ if and only if $p_1 \geq q_1$. From this, it also follows that if $\rho \not\succ \sigma$, then $p_1 < q_1$. Thus, we have that $\sigma \succ \rho$ instead. Notice that $p_1 = q_1$ does not necessarily mean that both states are the same; they could still have a different spectral decomposition.

Using this information, we can show that single-qubit state transitions with trivial Hamiltonians can never super-activate each other.

Lemma 1. *If ρ_1, ρ_2, σ_1 and σ_2 are 2-dimensional quantum states with trivial Hamiltonians, such that $\rho_1 \not\succ \sigma_1$ and $\rho_2 \not\succ \sigma_2$, then it follows that $\rho_1 \otimes \rho_2 \not\succ \sigma_1 \otimes \sigma_2$.*

Proof. Let $\{p_i^1\}$ be the ordered eigenvalues of ρ_1, $\{p_i^2\}$ be the ordered eigenvalues of ρ_2, $\{q_i^1\}$ be the ordered eigenvalues of σ_1 and $\{q_i^2\}$ be the ordered eigenvalues of σ_2, all in decreasing order. Furthermore, let $\{p_i\}$ be the ordered eigenvalues of $\rho_1 \otimes \rho_2$, and let $\{q_i\}$ be the ordered eigenvalues of $\sigma_1 \otimes \sigma_2$, again in decreasing order. Then, as we explained before, it follows from $\rho_1 \not\succ \sigma_1$ that $p_1^1 < q_1^1$. Similarly, it follows from $\rho_2 \not\succ \sigma_2$ that $p_1^2 < q_1^2$.

In order to show that $\rho_1 \otimes \rho_2 \not\succ \sigma_1 \otimes \sigma_2$, we will compare $\sum_{i=1}^k p_i$ with $\sum_{i=1}^k q_i$ for $k = 1$. Because p_i and q_i are products of the form $p_i^1 p_j^2$ with $i, j = \{1, 2\}$, it is easy to see that the largest eigenvalue of the joint system is given by $p_1^1 p_1^2$. Similarly, the largest eigenvalue of $\sigma_1 \otimes \sigma_2$ is given by $q_1^1 q_1^2$. This gives us that

$$\sum_{i=1}^{1} p_i = p_1 = p_1^1 p_1^2 \tag{64}$$

$$< q_1^1 q_1^2 = \sum_{i=1}^{1} q_i. \tag{65}$$

Thus, it follows that $\rho_1 \otimes \rho_2 \not\succ \sigma_1 \otimes \sigma_2$, which means that a transition is impossible. □

With this we conclude our analysis on 2-dimensional states.

3.1.2 Combining transitions

In order to find examples of super-activation, it will be useful to have some knowledge on which states not to combine. The following theorem will be useful in that respect.

Theorem 2. *Let ρ_1 and σ_1 be n-dimensional quantum states with trivial Hamiltonians, and let ρ_2 and σ_2 be m-dimensional quantum states with trivial Hamiltonians. If $\rho_1 \succ \sigma_1$ and $\rho_2 \succ \sigma_2$, then $\rho_1 \otimes \rho_2 \succ \sigma_1 \otimes \sigma_2$.*

Proof. Let p_i^1 be the ordered eigenvalues of ρ_1, such that $p_1 \geq \ldots \geq p_n$. Similarly, let p_i^2 be the eigenvalues of ρ_2, q_i^1 the eigenvalues of σ_1 and q_i^2 the eigenvalues of σ_2, all in decreasing order. Assume that $\rho_1 \succ \sigma_1$, and that $\rho_2 \succ \sigma_2$. Then, for every $1 \leq k \leq n$, we have that $\sum_{i=1}^k p_i^1 \geq \sum_{i=1}^k q_i^1$. For ρ_2 and σ_2, the same holds: $\sum_{i=1}^k p_i^2 \geq \sum_{i=1}^k q_i^2$ for every $1 \leq k \leq m$.

The eigenvalues of $\rho_1 \otimes \rho_2$ are given by $p^1_i p^2_j$ for $i = 1, \dots, n$ and $j = 1, \dots, m$, and the eigenvalues of $\sigma_1 \otimes \sigma_2$ are given by $q^1_i q^2_j$ for$i = 1, \dots, n$ and $j = 1, \dots, m$. For $\rho_1 \otimes \rho_2$, we will denote the k-th biggest eigenvalue by p_k, and for $\sigma_1 \otimes \sigma_2$, we will denote the k-th biggest eigenvalue by q_k. We need to show that for every $1 \leq k \leq nm$, $\sum_{i=1}^k p_i \geq \sum_{i=1}^k q_i$ holds. To show this, we first define

$$w_\rho(i,j,k) = \begin{cases} 1 : & p^1_i p^2_j \text{ is one of the k largest eigenvalues of } \rho \\ 0 : & \text{otherwise} \end{cases} \tag{66}$$

$$w_\sigma(i,j,k) = \begin{cases} 1 : & p^1_i p^2_j \text{ is one of the k largest eigenvalues of } \sigma \\ 0 : & \text{otherwise} \end{cases} . \tag{67}$$

These functions tell us which $p^1_i p^2_j$ and $q^1_i q^2_j$ are included in the summation. This will allow us to rewrite majorization, such that

$$\begin{aligned} \sum_{i=1}^k p_i &= \sum_{i=1}^n \sum_{j=1}^m p^1_i p^2_j w_\rho(i,j,k) && (68) \\ &\geq \sum_{i=1}^n \sum_{j=1}^m p^1_i p^2_j w_\sigma(i,j,k). && (69) \\ & && (70) \end{aligned}$$

The first equation sums over the k largest eigenvalues of $\rho_1 \otimes \rho_2$. In the second equation, we substitute some of these eigenvalues for different eigenvalues of $\rho_1 \otimes \rho_2$. Because these different eigenvalues are smaller, the value of the sum can only decrease.

Next, we define

$$f_\sigma(j,k) = \sum_{i=1}^n w_\sigma(i,j,k) \tag{71}$$

$$g_\sigma(i,k) = \sum_{j=1}^m w_\sigma(i,j,k). \tag{72}$$

Notice that if $p^1_i p^2_j$ is one of the k largest eigenvalues of $\rho_1 \otimes \rho_2$, then for all $m, n \geq 0$, $p^1_{i-m} p^2_{j-n}$ is one of the k largest eigenvalues of $\rho_1 \otimes \rho_2$ as well. Using this fact combined with the previously defined functions, we can rewrite the summation in a more convenient way, such that

$$\sum_{i=1}^{n}\sum_{j=1}^{m}p_i^1p_j^2w_\sigma(i,j,k) = \sum_{i=1}^{n}\sum_{j=1}^{g_\sigma(i,k)}p_i^1p_j^2 \tag{73}$$

$$= \sum_{i=1}^{n}p_i^1\sum_{j=1}^{g_\sigma(i,k)}p_j^2 \tag{74}$$

$$\geq \sum_{i=1}^{n}p_i^1\sum_{j=1}^{g_\sigma(i,k)}q_j^2. \tag{75}$$

$$\tag{76}$$

Here, the inequality follows from the fact that ρ_2 majorizes σ_2. We can now switch back to using $w_\sigma(i,j,k)$, and swap the order of the summation. This yields

$$\sum_{i=1}^{n}p_i^1\sum_{j=1}^{g_\sigma(i,k)}q_j^2 = \sum_{i=1}^{n}\sum_{j=1}^{m}p_i^1q_j^2w_\sigma(i,j,k) \tag{77}$$

$$= \sum_{j=1}^{m}\sum_{i=1}^{n}p_i^1q_j^2w_\sigma(i,j,k). \tag{78}$$

We can now do the same as we did before, but with $f_\sigma(j,k)$ instead of $g_\sigma(i,k)$. This gives us that

$$\sum_{j=1}^{m}\sum_{i=1}^{n}p_i^1q_j^2w_\sigma(i,j,k)s = \sum_{j=1}^{m}\sum_{i=1}^{f_\sigma(j,k)}p_i^1q_j^2 \tag{79}$$

$$= \sum_{j=1}^{m}q_j^2\sum_{i=1}^{f_\sigma(j,k)}p_i^1 \tag{80}$$

$$\geq \sum_{j=1}^{m}q_j^2\sum_{i=1}^{f_\sigma(j,k)}q_i^1. \tag{81}$$

The inequality holds because ρ_1 majorizes σ_1. We can express this in terms of q_i, such that

$$\sum_{j=1}^{m}q_j^2\sum_{i=1}^{f_\sigma(j,k)}q_i^1 = \sum_{i=1}^{n}\sum_{j=1}^{m}q_i^1q_j^2w_\sigma(i,j,k) \tag{82}$$

$$= \sum_{i=1}^{k}q_i. \tag{83}$$

The result is that for all $1 \leq k \leq nm$,

$$\sum_{i=1}^{k} p_i \geq \sum_{i=1}^{k} q_i, \tag{84}$$

and thus $\rho_1 \otimes \rho_2$ majorizes $\sigma_1 \otimes \sigma_2$. $\square$

This theorem can be particularly useful when trying to construct examples of super-activation, as we will show in the next section.

3.1.3 Constructing examples of super-activation

So far we have only found some restrictions on super-activation. It would be nice if we could also say something about the possibility of super-activation. In this section, we will give a way to construct examples of super-activation for some states with trivial Hamiltonians in any dimension.

The goal is to find for a given ρ_1 and σ_1 such that $\rho_1 \not\rightarrow \sigma_1$, ρ_2 and σ_2 such that$\rho_2 \not\rightarrow \sigma_2$ and $\rho_1 \otimes \rho_2 \rightarrow \sigma_1 \otimes \sigma_2$. As we showed in theorem 2, combining the transitions $\rho_1 \rightarrow \sigma_1$ and $\rho_2 \rightarrow \sigma_2$ yields $\rho_1 \otimes \rho_2 \rightarrow \sigma_1 \otimes \sigma_2$. However, this cannot directly be used to construct examples of super-activation.

Instead, we can combine two different transitions $\rho_1 \rightarrow \sigma_2$ and $\rho_2 \rightarrow \sigma_1$. This gives a new transition $\rho_2 \otimes \rho_1 \rightarrow \sigma_1 \otimes \sigma_2$. Because switching the order of the tensor products does not change the ordered eigenvalues, this also means that $\rho_1 \otimes \rho_2 \rightarrow \sigma_1 \otimes \sigma_2$. If in addition $\rho_1 \not\rightarrow \sigma_1$ and $\rho_2 \not\rightarrow \sigma_2$, this would be an example of a super-activated transition.

To use this information to construct examples of super-activation, we will need to slightly restrict ρ_1: if $\sigma_1 \succ \rho_1$, then we have that $\rho_2 \succ \sigma_1 \succ \rho_1 \succ \sigma_2$ which would mean that this is not an example of super-activation. Thus, we will restrict ρ_1 and σ_1 to be incomparable.

Theorem 3. *Let ρ_1 and σ_1 be d-dimensional quantum states with trivial Hamiltonians, such that $\rho_1 \not\succ \sigma_1$ and $\sigma_1 \not\succ \rho_1$. Then we can find ρ_2 and σ_2 such that $\rho_1 \otimes \rho_2 \succ \sigma_1 \otimes \sigma_2$. In particular, we can find $\rho_2 \not\succ \sigma_2$ for which the joint transition is possible.*

Proof. To prove that this is always possible, we will try to construct ρ_2 and σ_2 such that $\rho_2 \succ \sigma_1$ and $\rho_1 \succ \sigma_2$, while ensuring that $\rho_2 \not\succ \sigma_2$.

Let d be the dimension of ρ_1 and σ_1, and let $\{p_i^1\}$ and $\{q_i^1\}$ be the ordered eigenvalues of ρ_1 and σ_1 respectively. Then, because $\sigma_1 \not\succ \rho_1$, there exists at least one $k \in \mathbb{N}$ for which it holds that

$$\sum_{i=1}^{k} p_i^1 > \sum_{i=1}^{k} q_i^1. \tag{85}$$

Using this information, we can determine the eigenvalues of ρ_2 and σ_2. First, we define

$$\epsilon \equiv \frac{1}{3} \max_{k\in\mathbb{N}} \left(\sum_{i=1}^{k} p_i^1 - \sum_{i=1}^{k} q_i^1 \right) = \frac{1}{3} \left(\sum_{i=1}^{N} p_i^1 - \sum_{i=1}^{N} q_i^1 \right), \tag{86}$$

where we will denote the index for which this maximum occurred by N. Next, we determine $M \in \mathbb{N}$ such that

$$\sum_{i=M+1}^{d} q_i^1 < \epsilon \leq \sum_{i=M}^{d} q_i^1. \tag{87}$$

This M tells us how many eigenvalues at the tail of σ_1 we have to adjust in order to create a normalized ρ_2. With knowledge of M, we can define the eigenvalues of ρ_2 to be

$$p_i^2 = \begin{cases} q_i^1 + \epsilon & \text{if } i = 1 \\ q_i^1 & \text{if } 1 < i < M \\ q_i^1 - \epsilon + \sum_{j=M+1}^{d} q_i^1 & \text{if } i = M \\ 0 & \text{otherwise.} \end{cases} \tag{88}$$

This gives us the normalized state ρ_2 for which we have that

$$\sum_{i=1}^{k} p_i^2 \geq \sum_{i=1}^{k} q_i^1, \forall k \in \mathbb{N}. \tag{89}$$

And thus, $\rho_2 \succ \sigma_1$.

We will define σ_2 in a similar way. We will take the eigenvalues of ρ_1, and change them in such a way that $\rho_1 \succ \sigma_2$. We do need to be slightly more careful, however, in order to make sure that the order of the eigenvalues does not change. First, we determine $N_1 \in \mathbb{N}$ such that

$$\sum_{i=1}^{N_1-1} \left(p_i^1 - p_{N_1}^1 \right) < \epsilon \leq \sum_{i=1}^{N_1} \left(p_i^1 - p_{N_1+1}^1 \right). \tag{90}$$

and $N_2 \in \mathbb{N}$ such that

$$\sum_{i=N_2+1}^{d} \left(p_{N_2}^1 - p_i^1 \right) < \epsilon \leq \sum_{i=N_2}^{d} \left(p_{N_2-1}^1 - p_i^1 \right). \tag{91}$$

Then, N_1 and N_2 tell us how many eigenvalues we have to adjust to avoid changing the order of the eigenvalues. We can now determine the eigenvalues of σ_2. We define these by

$$q_i^2 = \begin{cases} \frac{1}{N_1}\left(-\epsilon + \sum_{i=1}^{N_1} p_i^1\right) & \text{if } i \leq N_1 \\ \frac{1}{d+1-N_2}\left(\epsilon + \sum_{i=N_2}^{d} p_i^1\right) & \text{if } i \geq N_2 \\ p_i^1 & \text{otherwise.} \end{cases} \tag{92}$$

This gives us another normalized state for which we have that

$$\sum_{i=1}^{k} p_i^1 \geq \sum_{i=1}^{k} q_i^2, \forall k \in \mathbb{N}. \tag{93}$$

And thus, $\rho_1 \succ \sigma_2$. Because also $\rho_2 \succ \sigma_1$, the joint transition is possible. Next, we will show that $\rho_2 \not\succ \sigma_2$, by looking at majorization at index N. To do this, we first determine the relation between M, N_1, N_2 and M.

Recall that at index N, we have that

$$3\epsilon = \sum_{i=1}^{N} p_i^1 - \sum_{i=1}^{N} q_i^1. \tag{94}$$

We start by considering M and N. Because the eigenvalues are normalized, we have that

$$\sum_{i=N+1}^{d} q_i^1 = \sum_{i=1}^{d} q_i^1 - \sum_{i=1}^{N} q_i^1 \tag{95}$$

$$= 1 - \sum_{i=1}^{N} q_i^1. \tag{96}$$

Combining this with equation 94 yields

$$\sum_{i=N+1}^{d} q_i^1 = 3\epsilon + 1 - \sum_{i=1}^{N} p_i^1 \tag{97}$$

$$> \epsilon. \tag{98}$$

If we compare this to our choice of M, which was

$$\sum_{i=M+1}^{d} q_i^1 < \epsilon \leq \sum_{i=M}^{d} q_i^1, \tag{99}$$

we get that $N < M$. We can do something similar for N_1 and N_2. We have that

$$\sum_{i=1}^{N}\left(p_i^1 - p_{N+1}^1\right) = \sum_{i=1}^{N} p_i^1 - N p_{N+1}^1 \tag{100}$$

$$= 3\epsilon + \sum_{i=1}^{N} q_i^1 - N p_{N+1}^1, \tag{101}$$

where we again used the fact that the eigenvalues are normalized. Combining this with equation 94 yields

$$\sum_{i=1}^{N}\left(p_i^1 - p_{N+1}^1\right) > 3\epsilon + \sum_{i=1}^{N} q_i^1 - N q_{N+1}^1 \tag{102}$$

$$= 3\epsilon + \sum_{i=1}^{N}\left(q_i^1 - q_{N+1}^1\right) \tag{103}$$

$$> \epsilon. \tag{104}$$

Comparing this to our choice of N_1, which was

$$\sum_{i=1}^{N_1-1}\left(p_i^1 - p_{N_1}^1\right) < \epsilon \leq \sum_{i=1}^{N_1}\left(p_i^1 - p_{N_1+1}^1\right), \tag{105}$$

we see that, $N_1 - 1 < N$, such that $N_1 \leq N$. Finally, for N_2 we have that

$$\sum_{i=N+1}^{d}\left(p_N^1 - p_i^1\right) = \sum_{i=1}^{d}\left(p_N^1 - p_i^1\right) - \sum_{i=1}^{N}\left(p_N^1 - p_i^1\right) \tag{106}$$

$$= (d-N)p_N^1 - 1 + \sum_{i=1}^{N} p_i^1, \tag{107}$$

because of normalization. Combining this with equation 94 gives us that

$$\sum_{i=N+1}^{d}\left(p_N^1 - p_i^1\right) = (d-N)p_N^1 - 1 + 3\epsilon + \sum_{i=1}^{N} q_i^1 \tag{108}$$

$$> (d-N)q_N^1 - 1 + 3\epsilon + \sum_{i=1}^{N} q_i^1 \tag{109}$$

$$= 3\epsilon + \sum_{i=1}^{d}\left(q_N^1 - q_i^1\right) - \sum_{i=1}^{N}\left(q_N^1 - q_i^1\right) \tag{110}$$

$$= 3\epsilon + \sum_{i=N+1}^{d}\left(q_N^1 - q_i^1\right) \tag{111}$$

$$> \epsilon. \tag{112}$$

If we compare the result with our definition of N_2, which was

$$\sum_{i=N_2+1}^{d} \left(p^1_{N_2} - p^1_i\right) < \epsilon \leq \sum_{i=N_2}^{d} \left(p^1_{N_2-1} - p^1_i\right), \tag{113}$$

We get that $N < N_2$. Thus, we have that $N < M$ and $N_1 \leq N < N_2$. With this in mind, we can consider majorization at index N. We have that

$$\begin{aligned}\sum_{i=1}^{N} q^2_i - \sum_{i=1}^{N} p^2_i &= \left(\sum_{i=1}^{N_1} q^2_i + \sum_{i=N_1+1}^{N} q^2_i\right) - \left(\sum_{i=1}^{1} p^2_i + \sum_{i=2}^{N} p^2_i\right) &(114)\\ &= \left(\sum_{i=1}^{N_1} \frac{1}{N_1}\left(\sum_{j=1}^{N_1} p^1_j - \epsilon\right) + \sum_{i=N_1+1}^{N} p^1_i\right) - \left(q^1_i + \epsilon + \sum_{i=2}^{N} q^1_i\right). &(115)\end{aligned}$$

Here, we have substituted q^2_i and p^2_i with their definitions. Moving ϵ out of the summations and swapping the order of the first summation yields

$$\begin{aligned}\sum_{i=1}^{N} q^2_i - \sum_{i=1}^{N} p^2_i &= \left(\sum_{j=1}^{N_1} \frac{1}{N_1} \sum_{i=1}^{N_1} p^1_j + \sum_{i=N_1+1}^{N} p^1_i\right) - \left(q^1_i + \sum_{i=2}^{N} q^1_i\right) - 2\epsilon &(116)\\ &= \left(\sum_{j=1}^{N_1} p^1_j + \sum_{i=N_1+1}^{N} p^1_i\right) - \sum_{i=1}^{N} q^1_i - 2\epsilon &(117)\\ &= \sum_{i=1}^{N} p^1_i - \sum_{i=1}^{N} q^1_i - 2\epsilon &(118)\\ &= \epsilon > 0, &(119)\end{aligned}$$

This means that $\rho_2 \not\succ \sigma_2$, and thus we have successfully constructed an example of super-activation for the initial transition $\rho_1 \rightarrow \sigma_1$. □

We will give an example to illustrate the procedure.

Example 3.1. Let ρ_1 and σ_1 be 4-dimensional quantum systems with trivial Hamiltonians. Let the eigenvalues of ρ_1 be given by $\{0.5, 0.2, 0.15, 0.15\}$, and let the eigenvalues of σ_1 be given by $\{0.4, 0.35, 0.15, 0.1\}$. Then, the first question that has to be answered, is if $\rho_1 \succ \sigma_1$, or if $\sigma_1 \succ \rho_1$. If neither are true, then we can apply our method to construct an example of super-activation.

We give the majorization-diagram of ρ_1 and σ_1 in figure 2.

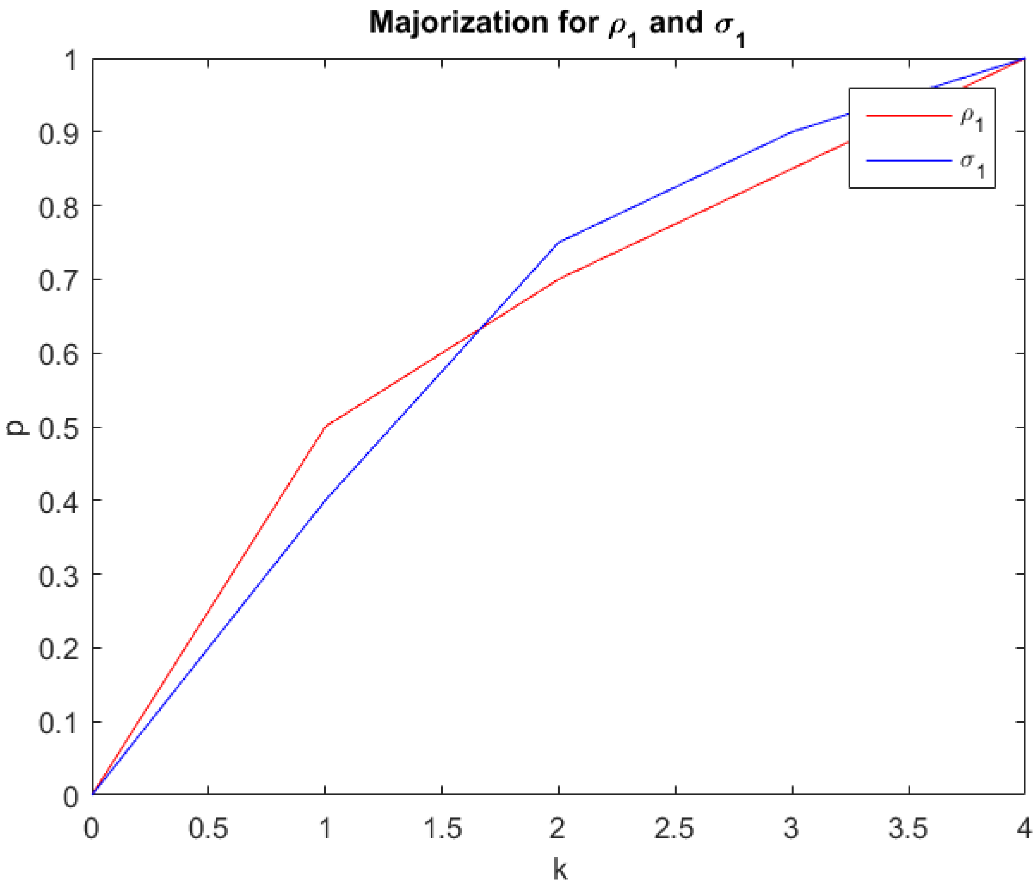

Figure 2: The majorization diagram of ρ_1 and σ_1. Since the diagrams intersect, the states are incomparable.

Clearly, ρ_1 and σ_1 are incomparable, and thus we can proceed with using our method. We start by finding the value of ϵ. Notice that the maximum difference of the two curves occurs at $k = 1$, such that $\epsilon = \frac{1}{3}\left(p_1^1 - q_1^1\right) = \frac{1}{30}$.

Next, we determine the values of M, N_1 and N_2. We find that $M = 4$, $N_1 = 1$ and $N_2 = 3$. Thus, for ρ_2 we only have to modify the first and the last eigenvalues of σ_1. For σ_2 we have to modify the first and the last two eigenvalues of ρ_1. We have that

$$p^2 = \{0.4333, 0.3500, 0.1500, 0.0667\} \tag{120}$$

$$q^2 = \{0.4667, 0.2000, 0.1667, 0.1667\}. \tag{121}$$

In figure 3, we give the majorization diagram of the four individual states to illustrate how the new curves compare to the old.

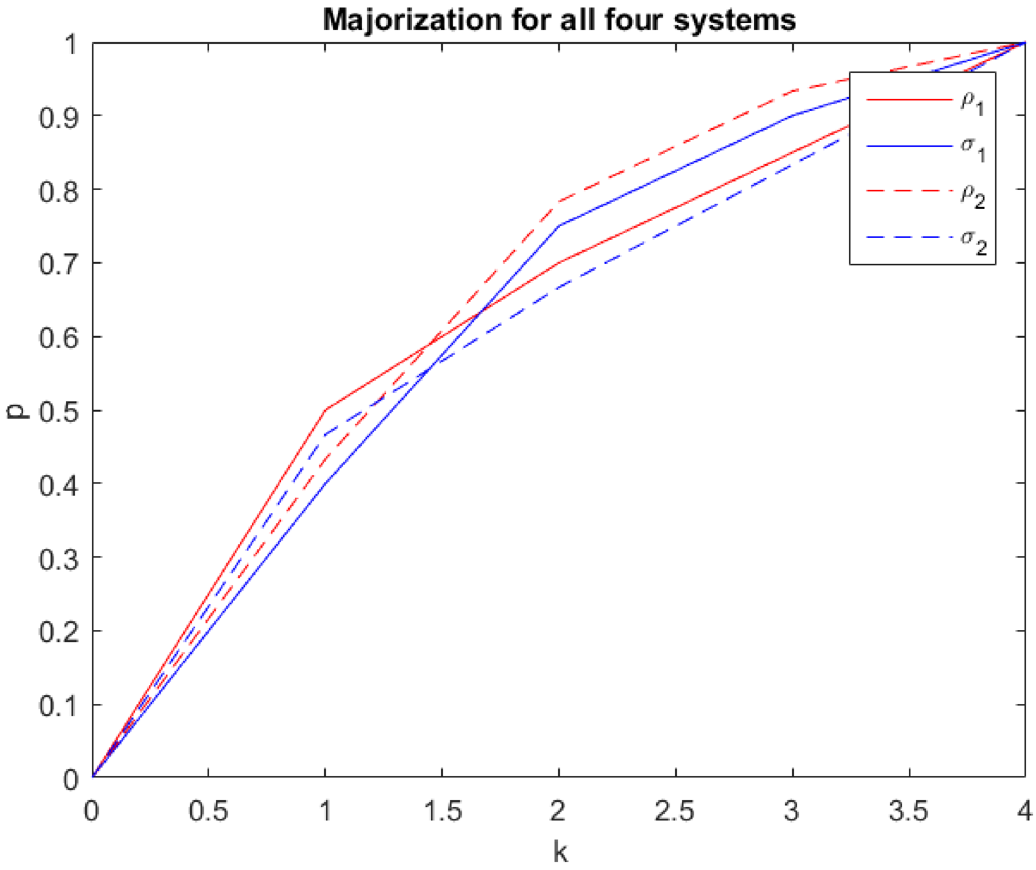

Figure 3: The majorization diagram of ρ_1, ρ_2, σ_1 and σ_2. The diagrams of ρ_2 and σ_2 intersect, which means that the states are incomparable. A transition from ρ_2 to σ_2 is therefore not possible by thermal operation.

finally, we verify that $\rho_1 \otimes \rho_2 \succ \sigma_1 \otimes \sigma_2$. In figure 4 we give the majorization diagram of these states.

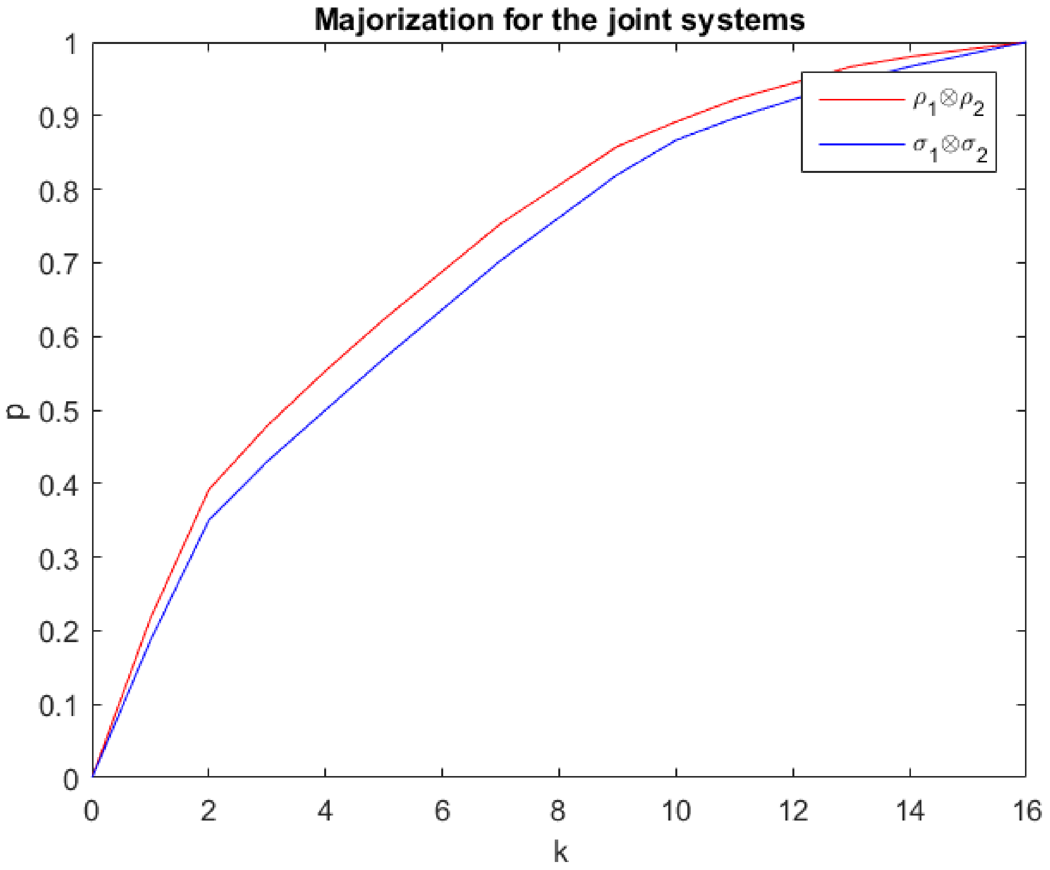

Figure 4: The majorization diagram of $\rho_1 \otimes \rho_2$ and $\sigma_1 \otimes \sigma_2$. It is clear that the diagram of the former lies above the diagram of the latter, such that a transition between the two is possible.

Since neither $\rho_1 \to \sigma_1$ nor $\rho_2 \to \sigma_2$, while the joint transition $\rho_1 \otimes \rho_2 \to \sigma_1 \otimes \sigma_2$ is possible, we have successfully constructed an example of super-activation.

3.1.4 Self-activation

As we explained in the background section, self-activation is the special case of super-activation, where we combine multiple instances of the same transitions. When the Hamiltonians are trivial, a transition is self-activated if $\rho \not\succ \sigma$, but there exists an $n \in \mathbb{N}$ such that $\rho^{\otimes n} \succ \sigma^{\otimes n}$. In this subsection, we will give the results that are related to this phenomenon.

To analyze self-activation, we will start by giving some general constraints on the states. Let ρ and σ be d-dimensional quantum systems, such that $\rho \not\succ \sigma$. Since we are looking at the case where $\rho^{\otimes n} \succ \sigma^{\otimes n}$, we can already find a restriction to ρ and σ: $\sigma \not\succ \rho$ has to hold. Otherwise, we can simply apply theorem 2 to the system multiple times, and find that $\sigma^{\otimes n} \succ \rho^{\otimes n}$. As we explained before, this implies that $\rho^{\otimes n}$ and $\sigma^{\otimes n}$ have the same ordered eigenvalues. However, since ρ is unequal to σ, this cannot be the case. Thus, ρ and σ have to be incomparable.

This brings up a new question. Since ρ and σ are assumed to be incomparable, it is no longer clear what differentiates the two. Maybe we could find some $N_1 \in \mathbb{N}$ such that $\rho^{\otimes N_1} \rightarrow \sigma^{\otimes N_1}$, and maybe we can find a $N_2 \in \mathbb{N}$ such that $\sigma^{\otimes N_2} \rightarrow \rho^{\otimes N_2}$. Maybe we can even find both N_1 and N_2 for the same ρ and σ, though that would have strange consequences.

In order to examine this question further, we will first try to find some necessary conditions for self-activation.

Theorem 4. *Let ρ and σ be d-dimensional systems, with eigenvalues p_i and q_i respectively, such that $\rho \not\succ \sigma$. If $\sum_{i=1}^{N} p_i < \sum_{i=1}^{N} q_i$ for some N, then the existence of $n_1 < N < n_2$, with $n_1, n_2 \in \mathbb{N}$ such that $\sum_{i=1}^{n_1} p_i > \sum_{i=1}^{n_1} q_i$ and $\sum_{i=1}^{n_2} p_i > \sum_{i=1}^{n_2} q_i$ is necessary for self activation to occur.*

Proof. We will prove this by contradiction. We first choose n, the number of copies of ρ, arbitrarily. This already defines the eigenvalues of both $\rho^{\otimes n}$ and $\sigma^{\otimes n}$. We will denote the ordered eigenvalues of $\rho^{\otimes n}$ and $\sigma^{\otimes n}$ by $\hat{p}_i$ and $\hat{q}_i$ respectively, such that $\hat{p}_1 \geq \ldots \geq \hat{p}_{d^n}$ and $\hat{q}_1 \geq \ldots \geq \hat{q}_{d^n}$. Each of these eigenvalues can be written as a product of p_i or q_i. In order to write them as products, we will use the following notation.

$$p_{\vec{a}} = \prod_{i=1}^{n} p_{a_i} \tag{122}$$

$$q_{\vec{a}} = \prod_{i=1}^{n} q_{a_i} \tag{123}$$

Here, $\vec{a}$ is an n-dimensional vector with entries $a_i \in \{1, \ldots, d\}$. Furthermore, we will define sums over vectors of indices $\sum_{\vec{a}=\vec{x}}^{\vec{y}} f(\vec{a})$ to iterate over all $\vec{a}$ such that $a_i \in \{x_i, \ldots, y_i\}$ for all i.

First, we assume that no $n_1 < N$ exists for which $\sum_{i=1}^{n_1} p_i > \sum_{i=1}^{n_1} q_i$. If we then consider majorization for the index k for which $p_1^{d-1} p_N$ is the k-th largest eigenvalue of $\rho^{\otimes n}$, we will find that the transition is impossible. Since $\rho^{\otimes n}$ has n eigenvalues with the value $p_1^{d-1} p_N$, there are multiple k that satisy our needs. We will choose k such that $\hat{p}_{k+1} < \hat{p}_k$, which means we consider all eigenvalues equal to $p_1^{d-1} p_N$.

So, we are to compare $\sum_{i=1}^{k} \hat{p}_i$ and $\sum_{i=1}^{k} \hat{q}_i$ for the fixed value of k. In order to write these sums in terms of products of p_i and q_i, we will define the following functions.

$$w_\rho(\vec{a}, k) = \begin{cases} 1 : p_{\vec{a}} \text{ is one of the } k \text{ largest eigenvalues of } \rho^{\otimes n} \\ 0 : \text{otherwise} \end{cases} \tag{124}$$

$$w_\sigma(\vec{a}, k) = \begin{cases} 1 : q_{\vec{a}} \text{ is one of the } k \text{ largest eigenvalues of } \sigma^{\otimes n} \\ 0 : \text{otherwise} \end{cases} \tag{125}$$

These functions are very similar to the functions we used in an earlier proof. They tell us which eigenvalues are among the k largest, allowing us to rewrite majorization as follows. We have that

$$\sum_{i=1}^{k} \hat{p}_i = \sum_{\vec{a}=(1,\ldots,1)}^{(d,\ldots,d)} w_\rho(\vec{a}, k) p_{\vec{a}} \tag{126}$$

$$= \sum_{\vec{a}=(1,\ldots,1)}^{(d,\ldots,d)} \left(w_\rho(\vec{a}, k) \prod_{i=1}^{n} p_{a_i} \right). \tag{127}$$

Next, we will multiply this expression by $\prod_{l=1}^{0} q_{a_l} = 1$, which yields

$$\sum_{i=1}^{k} \hat{p}_i = \sum_{\vec{a}=(1,\ldots,1)}^{(d,\ldots,d)} \left(w_\rho(\vec{a}, k) \prod_{i=1}^{n} p_{a_i} \right) \tag{128}$$

$$= \sum_{\vec{a}=(1,\ldots,1)}^{(d,\ldots,d)} \left(w_\rho(\vec{a}, k) \prod_{l=1}^{0} q_{a_l} \prod_{i=1}^{n} p_{a_i} \right). \tag{129}$$

We do this, because we want to eliminate all p_{a_i} from the expression. Having the equation in this form, will allow us to apply the following equation to it, repeatedly. We will use that for all $0 \le m < n$,

$$\sum_{\vec{a}=(1,\dots,1)}^{(d,\dots,d)}\left(w_\rho(\vec{a},k)\prod_{l=1}^{m}q_{a_l}\prod_{i=m+1}^{n}p_{a_i}\right)<\sum_{\vec{a}=(1,\dots,1)}^{(d,\dots,d)}\left(w_\rho(\vec{a},k)\prod_{l=1}^{m+1}q_{a_l}\prod_{i=m+2}^{n}p_{a_i}\right). \tag{130}$$

To show that this is the case, we will define a new function,

$$f_\rho(i,\vec{a},k)=\sum_{j=1}^{n}w_\rho((a_1,\dots,a_{i-1},j,a_{i+1},\dots,a_n),k), \tag{131}$$

where in the argument of w we changed the i-th entry of $\vec{a}$ to be equal to j. This function will tell us how many eigenvalues have all but the i-th index in common with the vector $\vec{a}$. it will help us to rewrite majorization further, giving us

$$\sum_{\vec{a}=(1,\dots,1)}^{(d,\dots,d)}\left(w_\rho(\vec{a},k)\prod_{l=1}^{m}q_{a_l}\prod_{i=m+1}^{n}p_{a_i}\right)=\sum_{\vec{a}=(1,\dots,1)}^{(d,\dots,1,\dots,d)}\left(\sum_{j=1}^{f_\rho(m+1,\vec{a},k)}p_j\prod_{l=1}^{m}q_{a_l}\prod_{i=m+2}^{n}p_{a_i}\right). \tag{132}$$

Here, the upper bound for $\vec{a}$ in the first summation on the right hand side is $(d,\dots,1,\dots,d)$. All but the $(m+1)$-th entry of this vector equal d, and the $(m+1)$-th entry equals 1. The summation on the left hand side iterates over far more vectors. On the right hand side, these vectors are taken into account by the second summation.

On the right hand side, we have a sum over products multiplied by p_j. Since these products are independent of j, we can move them outside of the sum, which yields

$$\sum_{\vec{a}=(1,\dots,1)}^{(d,\dots,d)}\left(w_\rho(\vec{a},k)\prod_{l=1}^{m}q_{a_l}\prod_{i=m+1}^{n}p_{a_i}\right)=\sum_{\vec{a}=(1,\dots,1)}^{(d,\dots,1,\dots,d)}\left(\prod_{l=1}^{m}q_{a_l}\prod_{i=m+2}^{n}p_{a_i}\sum_{j=1}^{f_\rho(m+1,\vec{a},k)}p_j\right). \tag{133}$$

Because of our assumption that no $n_1<N$ exists for which $\sum_{i=1}^{n_1}p_i>\sum_{i=1}^{n_1}q_i$, and because $f_\rho(m+1,\vec{a},k)\le N$, we have that

$$\sum_{i=1}^{f_\rho(m+1,\vec{a},k)}p_i\le\sum_{i=1}^{f_\rho(m+1,\vec{a},k)}q_i. \tag{134}$$

For several $\vec{a}$, a strict inequality occurs: we chose k such that all $p_1^{d-1}p_N$ are present in the summation, which means that $f_\rho(m+1,\vec{a},k)$ reaches N at least once. For these $\vec{a}$, we have

$$\sum_{i=1}^{f_\rho(m+1,\vec{a},k)} p_i = \sum_{i=1}^{N} p_i \tag{135}$$

$$< \sum_{i=1}^{N} q_i \tag{136}$$

$$= \sum_{i=1}^{f_\rho(m+1,\vec{a},k)} q_i. \tag{137}$$

Combining this fact with equation 133, yields

$$\sum_{\vec{a}=(1,\dots,1)}^{(d,\dots,d)} \left(w_\rho(\vec{a},k) \prod_{l=1}^{m} q_{a_l} \prod_{i=m+1}^{n} p_{a_i} \right) < \sum_{\vec{a}=(1,\dots,1)}^{(d,\dots,1,\dots,d)} \left(\prod_{l=1}^{m} q_{a_l} \prod_{i=m+2}^{n} p_{a_i} \sum_{j=1}^{f_\rho(m+1,\vec{a},k)} q_j \right). \tag{138}$$

Now we only need to move the product back into the summation, and go back to using w_ρ. This gives us that

$$\sum_{\vec{a}=(1,\dots,1)}^{(d,\dots,d)} \left(w_\rho(\vec{a},k) \prod_{l=1}^{m} q_{a_l} \prod_{i=m+1}^{n} p_{a_i} \right) < \sum_{\vec{a}=(1,\dots,1)}^{(d,\dots,1,\dots,d)} \left(\sum_{j=1}^{f_\rho(m+1,\vec{a},k)} q_j \prod_{l=1}^{m} q_{a_l} \prod_{i=m+2}^{n} p_{a_i} \right) \tag{139}$$

$$= \sum_{\vec{a}=(1,\dots,1)}^{(d,\dots,d)} \left(w_\rho(\vec{a},k) \prod_{i=1}^{m+1} q_{a_i} \prod_{i=m+2}^{n} p_{a_i} \right). \tag{140}$$

We can now repeatedly apply this to equation 129, increasing the value every single time. Then, we find that

$$\sum_{i=1}^{k} \hat{p}_i = \sum_{\vec{a}=(1,\dots,1)}^{(d,\dots,d)} \left(w_\rho(\vec{a},k) \prod_{l=1}^{0} q_{a_l} \prod_{i=1}^{n} p_{a_i} \right) \tag{141}$$

$$< \sum_{\vec{a}=(1,\dots,1)}^{(d,\dots,d)} \left(w_\rho(\vec{a},k) \prod_{l=1}^{1} q_{a_l} \prod_{i=2}^{n} p_{a_i} \right) \tag{142}$$

$$< \dots \tag{143}$$

$$< \sum_{\vec{a}=(1,\dots,1)}^{(d,\dots,d)} \left(w_\rho(\vec{a},k) \prod_{l=1}^{n} q_{a_l} \prod_{i=n+1}^{n} p_{a_i} \right) \tag{144}$$

$$= \sum_{\vec{a}=(1,\dots,1)}^{(d,\dots,d)} \left(w_\rho(\vec{a},k) \prod_{l=1}^{n} q_{a_l} \right). \tag{145}$$

Using the fact that the q_i are the ordered eigenvalues of σ, we can see that

$$\sum_{i=1}^{k} q_i \geq \sum_{i=1}^{k} q_{j(i)}, \tag{146}$$

where $j(i)$ is an arbitrary bijection between $\{1, \ldots, d\}$ and $\{1, \ldots, d\}$. For an explicit proof of this, we refer to lemma 1.

Since the order of p_i and q_i might be different, we are essentially dealing with such a bijection. Thus, we have that

$$\sum_{i=1}^{k} \hat{p}_i < \sum_{\vec{a}=(1,\ldots,1)}^{(d,\ldots,d)} \left(w_\rho(\vec{a}, k) \prod_{l=1}^{n} q_{a_l} \right) \tag{147}$$

$$\leq \sum_{\vec{a}=(1,\ldots,1)}^{(d,\ldots,d)} \left(w_\sigma(\vec{a}, k) \prod_{l=1}^{n} q_{a_l} \right) \tag{148}$$

$$= \sum_{i=1}^{k} \hat{q}_i, \tag{149}$$

and thus, $\rho^{\otimes n} \not\succ \sigma^{\otimes n}$, rendering a transition impossible. As a direct result, the existence of n_1 is a necessity.

We can use a similar method to prove that the existence of n_2 is necessary; we first assume that n_2 does not exist. We then consider majorization for the index k for which p_N^d is the k-th largest eigenvalue of $\rho^{\otimes n}$. From here on, all previous equations hold, though some do for different reasons.

First of all, we no longer have that $f_\rho(m+1, \vec{a}, k) \leq N$. Instead, for all $\vec{a}$, $f_\rho(m + 1, \vec{a}, k) \geq N$. Fortunately, because of our assumption that no $n_2 > N$ exists for which $\sum_{i=1}^{n_1} p_i > \sum_{i=1}^{n_1} q_i$, this means that equation 134 still holds.

Secondly, because the eigenvalue p_N^d is the k-th largest eigenvalue, we still have that $f_\rho(m+1, \vec{a}, k) = N$ for some $\vec{a}$. Therefore, the strict inequality of equation 138 is still true.

This means that all equations untill 149 also still hold, and thus, $\rho^{\otimes n} \not\succ \sigma^{\otimes n}$, rendering a transition impossible. As a direct result, the existence of n_2 is a necessity as well. $\square$

We leave a few remarks before discussing the consequences of the theorem. First of all, since ρ can fail to majorize σ at multiple indices, we can apply the theorem to each of those indices separately. This means that, when N_1 and N_2 are the smallest and largest indices for which majorization fails respectively, the existence of $n_1 < N_1 \leq N_2 < n_2$ such that $\sum_{i=1}^{n_1} p_i > \sum_{i=1}^{n_1} q_i$ and $\sum_{i=1}^{n_2} p_i > \sum_{i=1}^{n_2} q_i$ is necessary for self-activation to occur.

This gives some mathematical meaning to the theorem. The conditions mean that both the 'head' and 'tail' of the thermo-majorization curve of ρ need to be above the curve of σ. Figure 5 illustrates this.

The theorem has some very important consequences, even though the conditions are not sufficient for self-activation to occur. First of all, these conditions are quite stringent. If two states are incomparable, they can still fail to meet the conditions, possibly in both directions: there exist ρ and σ that are incomparable, for which $\rho^{\otimes n} \not\succ \sigma^{\otimes n}$ and $\sigma^{\otimes n} \not\succ \rho^{\otimes n}$ for all $n \in \mathbb{N}$.

Another result of this theorem, is that we can say something about the dimension of the states for which self-activation occurs.

Corollary 1. *Let ρ and σ be d-dimensional systems with trivial Hamiltonians. Furthermore, let $\rho \not\succ \sigma$. Then, if $\rho^{\otimes n} \succ \sigma^{\otimes n}$ for some $n \in \mathbb{N}$, it must hold that $d > 3$.*

Proof. Since $\rho \not\succ \sigma$ and $\rho^{\otimes n} \succ \sigma^{\otimes n}$, this is a self-activated transition. Thus, the necessary conditions given in theorem 4 are met by ρ and σ.

Let N be an index for which ρ fails to majorize σ, such that $\sum_{i=1}^{N} p_i < \sum_{i=1}^{N} q_i$. Then, according to the necessary conditions, there must exist $n_1 < N$ for which $\sum_{i=1}^{n_1} p_i > \sum_{i=1}^{n_1} q_i$, and $N < n_2$ for which $\sum_{i=1}^{n_2} p_i > \sum_{i=1}^{n_2} q_i$. Because these indices are positive, we also have that $n_1 > 0$. Furthermore, because the states are normalized, $\sum_{i=1}^{d} p_i > \sum_{i=1}^{d} q_i$ can never hold. Thus, we have that $n_2 < d$. This yields

$$0 < n_1 < N < n_2 < d. \tag{150}$$

This is only possible if $d \geq 4$. In 2- and 3-dimensional systems, self activation can not happen. □

We will give an example to illustrate the conditions.

Example 3.2. Let ρ and σ be 4-dimensional systems with a trivial Hamiltonians. Let their eigenvalues be given by $p = \{0.53, 0.25, 0.2, 0.02\}$ and $q = \{0.4, 0.4, 0.1, 0.1\}$ respectively.

First of all, since the systems are 4-dimensional, self activation might be possible. We can apply the conditions of theorem 4 to the system, so we can possibly rule out self-activation. If the conditions are met, however, we will have to check majorization for multiple copies. In figure 5, we give the majorization diagram of ρ and σ. We will assess the conditions graphically.

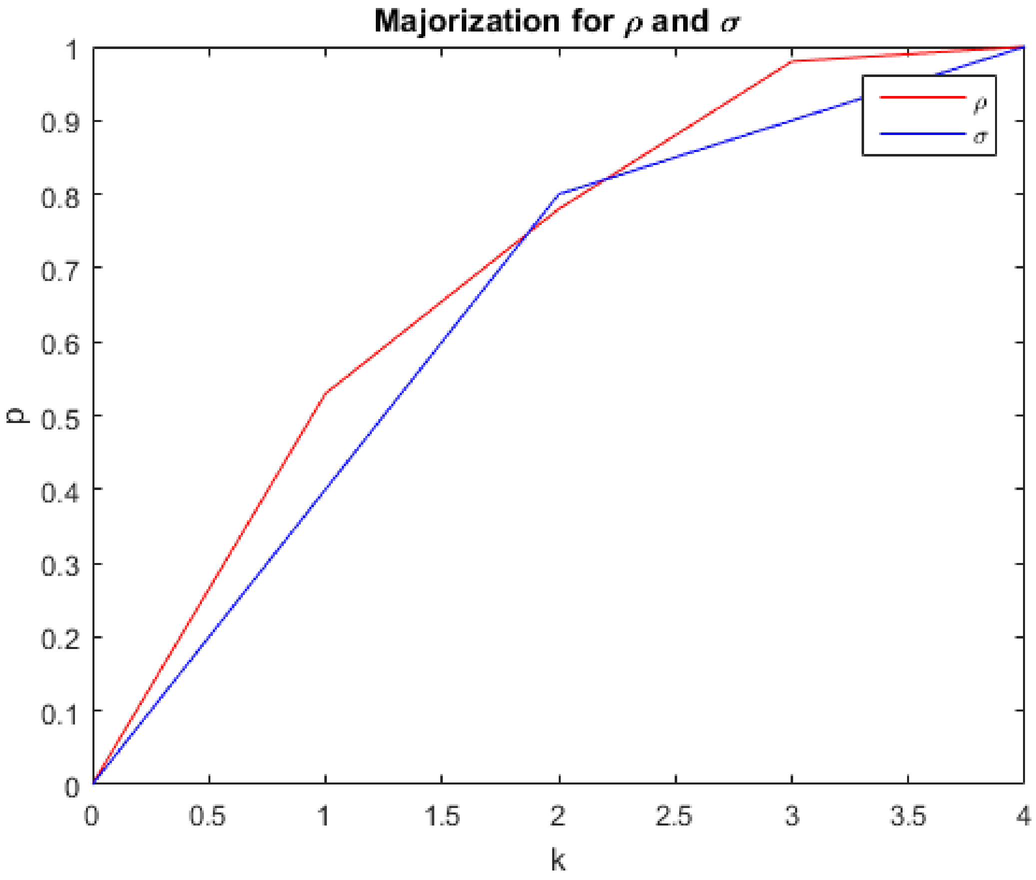

Figure 5: The majorization diagram of ρ and σ. it is clear that majorization fails at $k = 2$.

From the majorization-diagram of ρ and σ, it becomes clear that ρ fails to majorize σ at $k = 2$. Clearly, for $n_1 = 1$ and $n_2 = 3$ we have that $\sum_{i=1}^{n_1} p_i > \sum_{i=1}^{n_1} q_i$ and $\sum_{i=1}^{n_2} p_i > \sum_{i=1}^{n_2} q_i$. Thus, the conditions given in theorem 4 are met.

We can try to check for arbitrary values of n, the number of copies, if $\rho^{\otimes n} \succ \sigma^{\otimes n}$. We give the majorization diagram for $n = 2$ in figure 6.

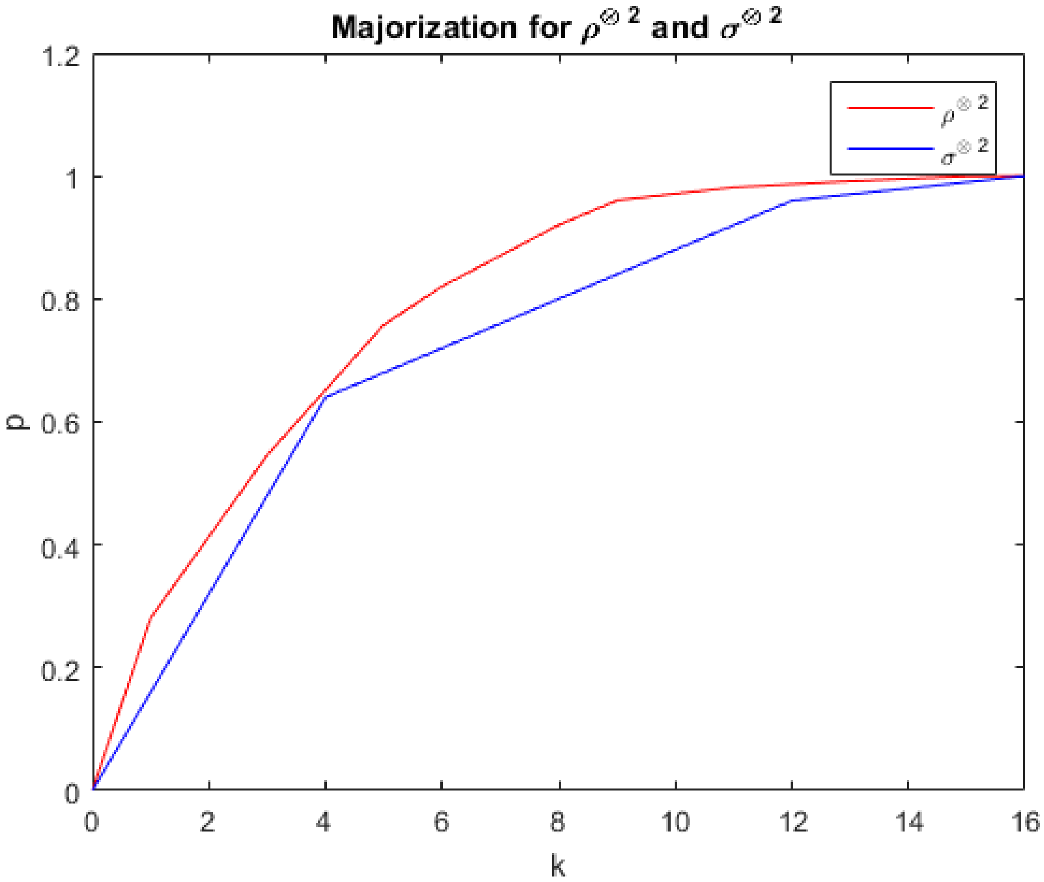

Figure 6: The majorization diagram of $\rho^{\otimes n}$ and $\sigma^{\otimes n}$. It is clear that the diagram of the former lies above the diagram of the latter.

Since the majorization diagram of $\rho^{\otimes 2}$ lies above the diagram of $\sigma^{\otimes 2}$, we have that the transition is possible, and thus this is an example of self-activation. Take in mind, however, that just because the conditions of theorem 4 were met by ρ and σ, self-activation did not necessarily have to occur; the conditions are only necessary.

Finally, we will show that there exists a catalyst that performs the transition $\rho \to \sigma$, as expected. If we consider the 2-dimensional system ω with a trivial Hamiltonian and eigenvalues $\{0.65, 0.35\}$, then the majorization diagram of $\rho \otimes \omega$ and $\sigma \otimes \omega$ is given in figure 7.

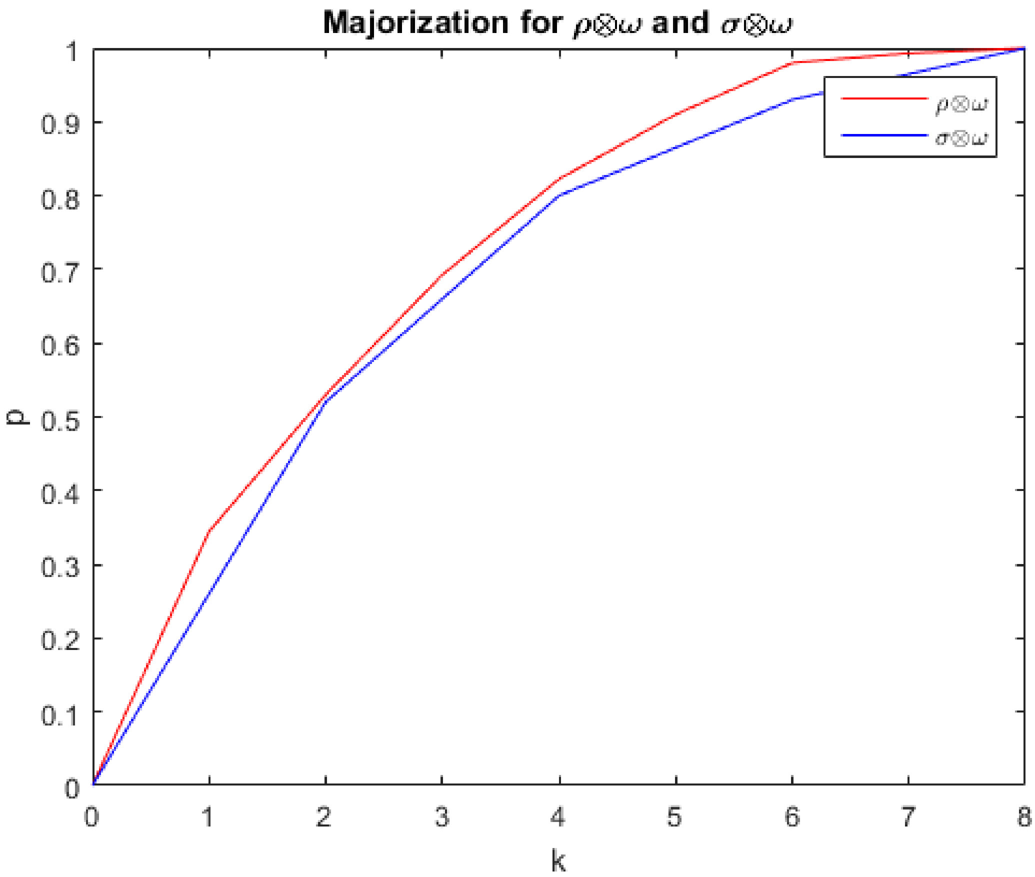

Figure 7: The majorization diagram of $\rho \otimes \omega$ and $\sigma \otimes \omega$. Clearly, the diagram of the former lies above the diagram of the latter.

Since the majorization diagram of $\rho\otimes\omega$ lies above the diagram of $\sigma\otimes\omega$, the transition is possible. This concludes the example.

The last consequence of theorem 4 is that we can answer the question we posed earlier: we cannot find both $N_1 \in \mathbb{N}$ and $N_2 \in \mathbb{N}$ such that $\rho^{\otimes N_1} \succ \sigma^{\otimes N_1}$ and $\sigma^{\otimes N_2} \succ \rho^{\otimes N_2}$. We explain this further in the next theorem.

Theorem 5. *Let ρ, σ be d-dimensional states with trivial Hamiltonians, such that there exists an $n \in \mathbb{N}$ for which $\rho^{\otimes n} \succ \sigma^{\otimes n}$, while $\rho \not\succ \sigma$. Then $\sigma^{\otimes m} \not\succ \rho^{\otimes m}$ for all $m \in \mathbb{N}$.*

Proof. Because $\rho^{\otimes n} \succ \sigma^{\otimes n}$ is possible, we have that the necessary conditions given by theorem 4 are met by ρ and σ.

Let N_1 and N_2 be the smallest and largest index for which ρ fails to majorize σ respectively. Then, because the necessary conditions are met, we have that there exist $n_2 < N_1 \leq N_2 < n_3$, with $n_2, n_3 \in \mathbb{N}$ such that $\sum_{i=1}^{n_2} p_i > \sum_{i=1}^{n_2} q_i$ and $\sum_{i=1}^{n_3} p_i > \sum_{i=1}^{n_3} q_i$.

Because N_1 was the smallest index for which ρ failed to majorize σ and N_2 was the largest, there can not exist $n_1 < n_2 < n_3 < n_4$, with $n_1, n_4 \in \mathbb{N}$ such that $\sum_{i=1}^{n_1} q_i > \sum_{i=1}^{n_1} p_i$ and $\sum_{i=1}^{n_4} q_i > \sum_{i=1}^{n_4} p_i$. Thus, by theorem 4, $\rho^{\otimes m} \to \sigma^{\otimes m}$ can not happen for any $m \in \mathbb{N}$. $\square$

3.2 Non-trivial Hamiltonians

In this section, we will give all the results that are related to super-activation with non-trivial Hamiltonians. We are again interested in transitions of the form $\rho_1 \otimes \rho_2 \to \sigma_1 \otimes \sigma_2$, while at the same time $\rho_1 \not\to \sigma_1$, and $\rho_2 \not\to \sigma_2$. We will assume that all states are block diagonal.

Some of the theorems we proved for the cases with trivial Hamiltonians, can most likely be extended to also hold for nontrivial cases. However, because comparing the thermo-majorization curves is far more complicated when the Hamiltonians are nontrivial, extending these theorems will probably not be easy. Instead of doing this, we will be giving some examples of the things that do change, while hinting at the extensions of these theorems.

In the previous section, we showed that when the Hamiltonians are trivial, qubits cannot super-activate each other. However, when the Hamiltonians are nontrivial, this is no longer the case. We will give an example to show this.

Example 3.3. let ρ_1, ρ_2, σ_1 and σ_2 be qubits with a nontrivial Hamiltonian. Let the exponent of the energy levels divided by the temperature, $e^{\beta E_i}$, of these systems be given by $\{1, 2\}$. Let the eigenvalues of the four states be given by $\{0.35, 0.65\}$, $\{0.85, 0.15\}$, $\{0.95, 0.05\}$ and $\{0.45, 0.55\}$ respectively. Notice that these eigenvalues are not β-ordered.

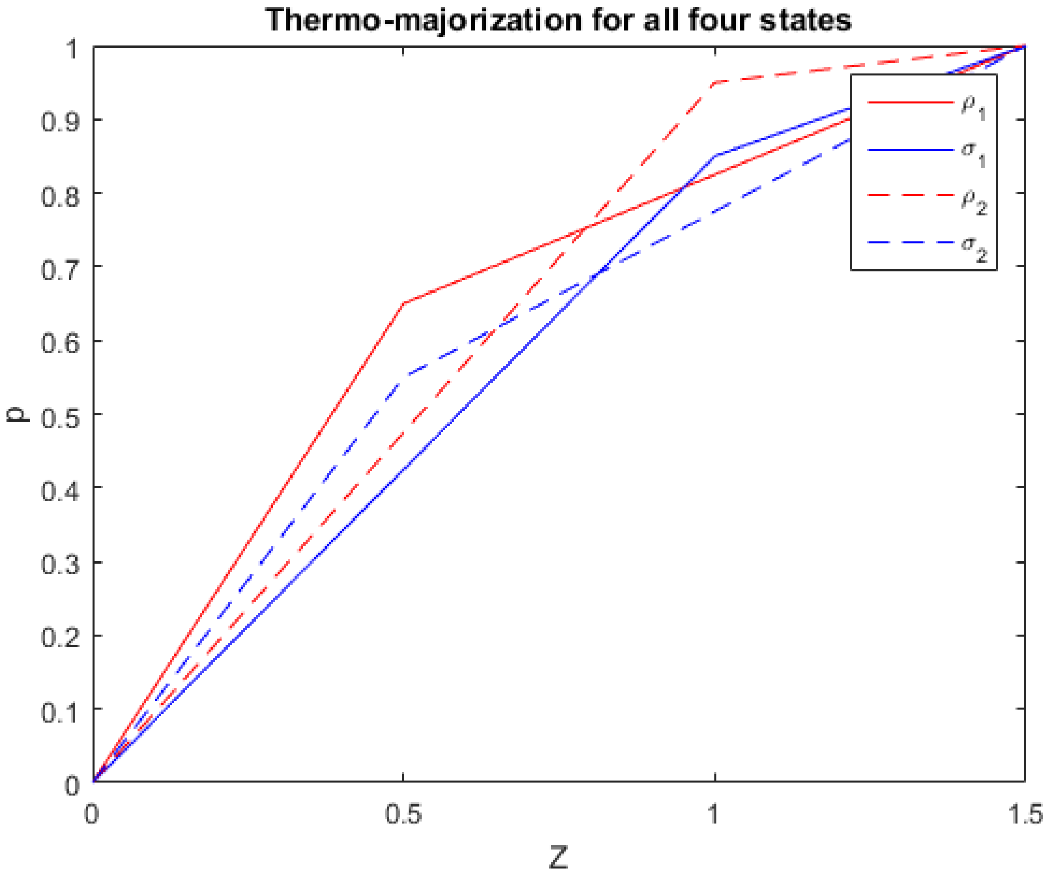

Figure 8: The thermo-majorization diagram of ρ_1, ρ_2, σ_1 and σ_2.

The thermo-majorization diagram of the four states is depicted in figure 8. The way these curves compare to each other may seem familiar. We actually applied our method of constructing examples of super-activation here to find an example: we picked the eigenvalues of ρ_2 and σ_2, such that the transitions $\rho_1 \to \sigma_2$ and $\rho_2 \to \sigma_1$ are both possible. Therefore, the joint transitions should also be possible.

To confirm that this is the case, we will also give the thermo-majorization diagrams of the joint systems. These can be seen in figure 9.

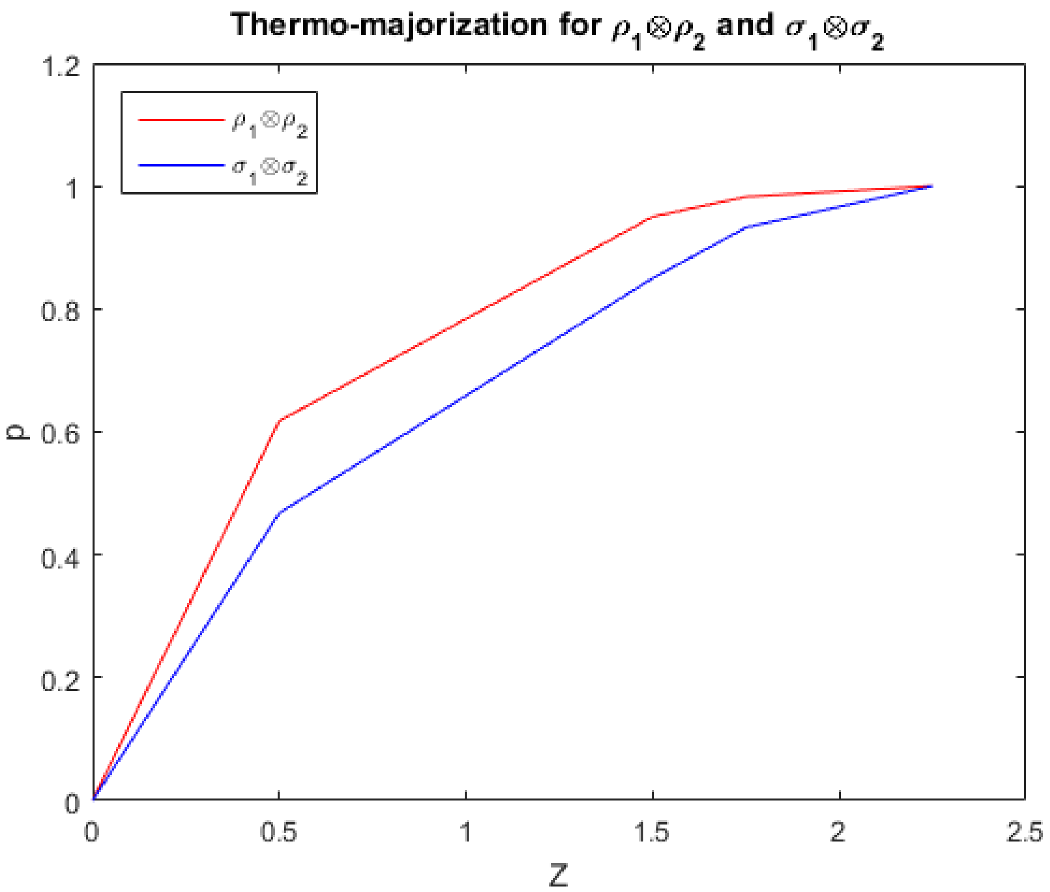

Figure 9: The thermo-majorization diagram of $\rho_1 \otimes \rho_2$ and $\sigma_1 \otimes \sigma_2$. Clearly, the former thermo-majorizes the latter.

Thus, we have found an example of super-activation in qubits.

For self-activation something similar changes. When the Hamiltonians are nontrivial, we can find examples of 3-dimensional states that can self-activate. We will again show this by giving such an example.

Example 3.4. Let ρ and σ be 3-dimensional quantum states. Let the exponent of the energy levels divided by the temperature, $e^{\beta E_i}$, of these systems be given by $\{1, 2, 8\}$. Let the eigenvalues of ρ and σ be given by $\{0.55, 0.1, 0.35\}$ and $\{0.35, 0.45, 0.2\}$ respectively. Notice that these eigenvalues are not β-ordered. The thermo-majorization diagram of ρ and σ is given in figure 10.

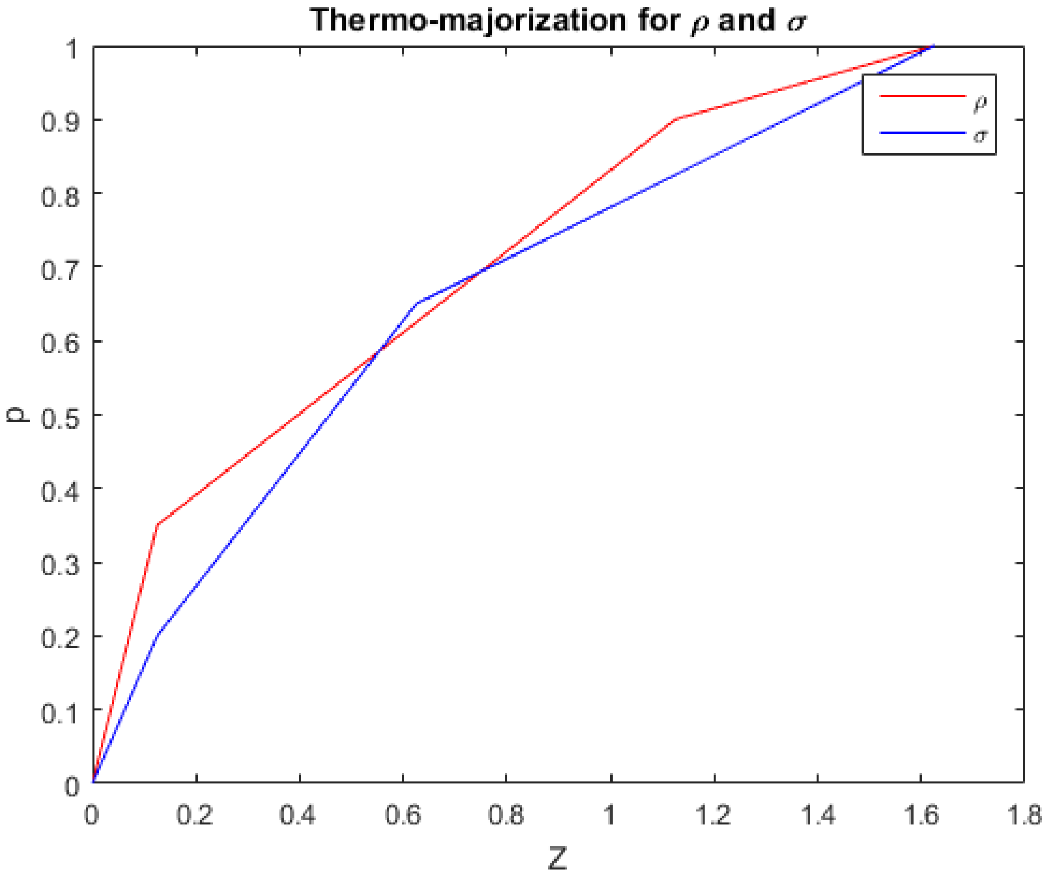

Figure 10: The thermo-majorization diagram of ρ and σ. Clearly, a transition $\rho \to \sigma$ is not possible.

From the thermo-majorization diagram it can be seen that the states are incomparable. Furthermore, the thermo-majorization curve of ρ exceeds the curve of σ both before and after the curve of σ exceeds the curve of ρ. This is very similar to the necessary conditions that we proved for trivial Hamiltonians.

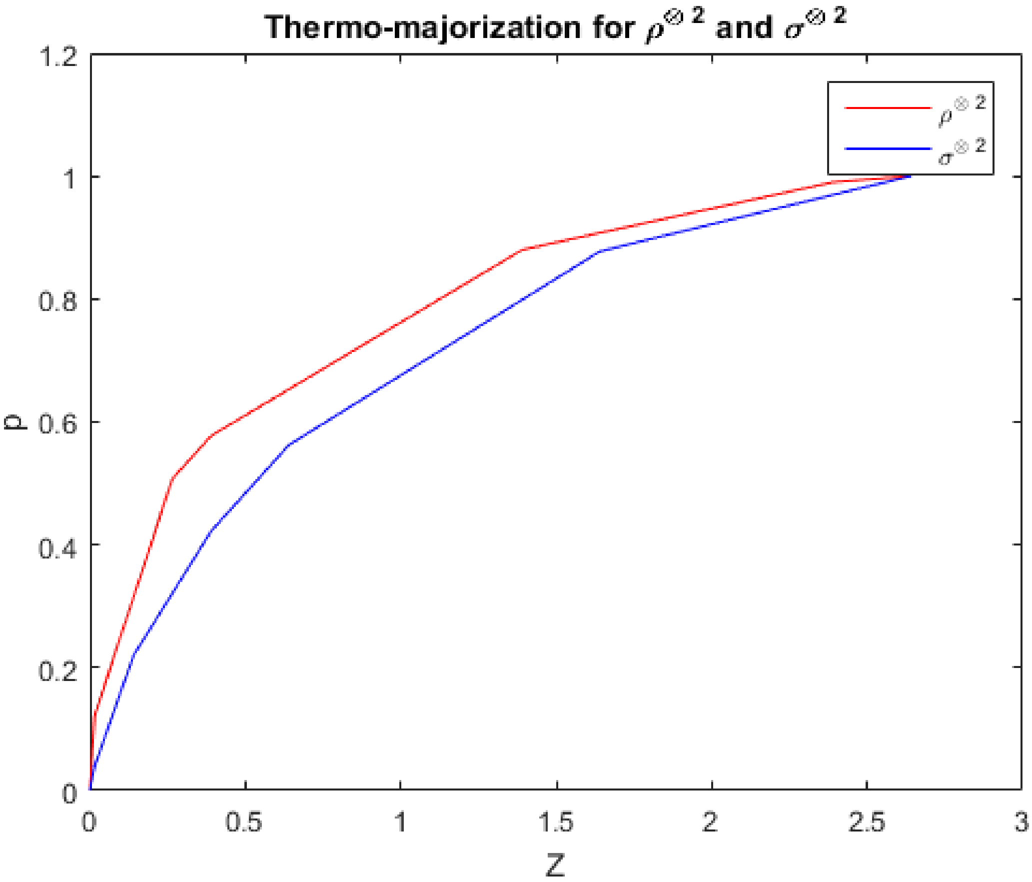

Figure 11: The thermo-majorization diagram of ρ and σ. Clearly, a transition $\rho^{\otimes 2} \to \sigma^{\otimes 2}$ is possible.

The thermo-majorization diagram of $\rho^{\otimes 2}$ and $\sigma^{\otimes 2}$ is given in figure 11. Clearly, the transition $\rho^{\otimes 2} \to \sigma^{\otimes 2}$ is possible. This shows that self-activation can occur in 3-dimensional states, if the Hamiltonians are nontrivial.

With this we conclude the results on nontrivial Hamiltonians. In the two examples we showed, we proved that two of the theorems we proved for trivial Hamiltonians, do not hold for nontrivial Hamiltonians. Furthermore, these examples suggest that theorem 2 and theorem 4 can be extended to the nontrivial case without too many problems.

4 Smoothing

Sometimes, one is interested in transitions where a small probability of failure is allowed. In other cases, getting into any state close to the target state is sufficient. This leads to the use of smoothing. Smoothing also allows us to verify if an infinite families of conditions on the Rényi entropies and divergences are met, by considering only two conditions on the smoothed entropies and divergences [2].

In this chapter, we give all the results related to the smoothed Rényi divergences. We first show that if these divergences decrease from a state ρ to a state σ, then the transition between two special states close to ρ and σ is possible. These special states are the steepest and flattest state, which we analyze after. We show that the steepest state exists for certain values of ϵ, and we show that the flattest state always exists.

4.1 Rényi Divergences

In this section, we will look at smoothing of the Rényi divergences. To recap, the smoothed Rényi divergences are defined as

$$D_\alpha^\epsilon(\rho||\tau) = \begin{cases} \min_{\tilde{\rho}} D_\alpha(\tilde{\rho}||\tau) & \text{if } \alpha < 0 \\ \max_{\tilde{\rho}} D_\alpha(\tilde{\rho}||\tau) & \text{if } 0 \leq \alpha \leq 1 \\ \min_{\tilde{\rho}} D_\alpha(\tilde{\rho}||\tau) & \text{if } \alpha > 1, \end{cases} \tag{151}$$

where optimization occurs over the states within an ϵ-ball around ρ. These states are given by

$$B^\epsilon(\rho) = \left\{ \tilde{\rho} : \frac{1}{2} \sum_i |p_i - \tilde{p}_i| \leq \epsilon \right\}. \tag{152}$$

Because these functions are defined differently for different regions, these smoothed divergences do not collectively correspond with the Rényi divergences of a particular state. However, in some scenarios we are still able to say something about transitions if we are given information about the smoothed divergences.

Recall that a transition $\rho \to \sigma$ between the block diagonal states ρ and σ is possible if and only if for $\alpha \in \mathbb{R}$,

$$D_\alpha(\rho||\tau) \geq D_\alpha(\sigma||\tau). \tag{153}$$

For the given ϵ-ball, we will define two special states: the steepest state and the flattest state.

Definition 4.1. The steepest state of ρ, ρ^{ϵ}_{steep}, is the state that can be transformed via thermal operations to any other state that is ϵ-close to ρ, such that for any $\tilde{\rho} \in B^{\epsilon}(\rho)$, $\rho^{\epsilon}_{steep} \to \tilde{\rho}$.

Definition 4.2. The flattest state of ρ, ρ^{ϵ}_{flat}, is the state that all other states that are ϵ-close to ρ can be transformed into via thermal operations, such that for any $\tilde{\rho} \in B^{\epsilon}(\rho)$, $\tilde{\rho} \to \rho^{\epsilon}_{flat}$.

Notice that these states may not exist; we are just introducing the concept here. We will look at the existence of these states later.

These states lead to the following observation. If the steepest state ρ^{ϵ}_{steep} exist for some ϵ, then we have that for all $\tilde{\rho}$ within the ϵ-ball,

$$D_{\alpha}(\rho^{\epsilon}_{steep}||\tau) \geq D_{\alpha}(\tilde{\rho}||\tau). \tag{154}$$

Similarly, if the flattest state exists, we have that for all $\tilde{\rho} \in B^{\epsilon}(\rho)$,

$$D_{\alpha}(\tilde{\rho}||\tau) \geq D_{\alpha}(\rho^{\epsilon}_{flat}||\tau). \tag{155}$$

These observations lead to the following theorem.

Theorem 6. *If for two states ρ and σ we have that $D^{\epsilon}_{\alpha}(\rho||\tau) \geq D^{\epsilon}_{\alpha}(\sigma||\tau)$ for all $\alpha \in \mathbb{R}$, then the steepest state of ρ, if it exists, can be transformed to the flattest state of σ.*

Proof. It is sufficient to show that $D_{\alpha}(\rho^{\epsilon}_{steep}||\tau) \geq D_{\alpha}(\sigma^{\epsilon}_{flat}||\tau)$ for all $\alpha \in \mathbb{R}$. Assume that $D^{\epsilon}_{\alpha}(\rho||\tau) \geq D^{\epsilon}_{\alpha}(\sigma||\tau)$. Then, for $\alpha < 0$ and for $\alpha > 1$ we have that

$$\min_{\tilde{\rho}} D_{\alpha}(\tilde{\rho}||\tau) = D^{\epsilon}_{\alpha}(\rho||\tau) \geq D^{\epsilon}_{\alpha}(\sigma||\tau) = \min_{\tilde{\sigma}} D_{\alpha}(\tilde{\sigma}||\tau), \tag{156}$$

from which it follows that

$$\begin{aligned} D_{\alpha}(\rho^{\epsilon}_{steep}||\tau) &\geq D_{\alpha}(\rho^{\epsilon}_{flat}||\tau) && (157)\\ &= \min_{\tilde{\rho}} D_{\alpha}(\tilde{\rho}||\tau) && (158)\\ &\geq \min_{\tilde{\sigma}} D_{\alpha}(\tilde{\sigma}||\tau) && (159)\\ &= D_{\alpha}(\sigma^{\epsilon}_{flat}||\tau). && (160) \end{aligned}$$

For $0 \leq \alpha \leq 1$ we have that

$$\max_{\tilde{\rho}} D_{\alpha}(\tilde{\rho}||\tau) = D^{\epsilon}_{\alpha}(\rho||\tau) \geq D^{\epsilon}_{\alpha}(\sigma||\tau) = \max_{\tilde{\sigma}} D_{\alpha}(\tilde{\sigma}||\tau). \tag{161}$$

Thus, it follows that

$$
\begin{aligned}
D_\alpha(\rho^\epsilon_{steep}||\tau) &= \max_{\tilde{\rho}} D_\alpha(\tilde{\rho}||\tau) && (162)\\
&\geq \max_{\tilde{\sigma}} D_\alpha(\tilde{\sigma}||\tau) && (163)\\
&= D_\alpha(\rho^\sigma_{steep}||\tau) && (164)\\
&\geq D_\alpha(\sigma^\epsilon_{flat}||\tau). && (165)
\end{aligned}
$$

Thus, for all $\alpha \in \mathbb{R}$ we have that $D_\alpha(\rho^\epsilon_{steep}||\tau) \geq D_\alpha(\sigma^\epsilon_{flat}||\tau)$. Therefore, the transition $\rho^\epsilon_{steep} \to \sigma^\epsilon_{flat}$ is possible by a catalytic thermal operation. □

This brings up an obvious question: when do these steepest and flattest states exist? We know that when the Hamiltonians are trivial, both the steepest and the flattest state exist for any $\epsilon > 0$. However, when the Hamiltonians are nontrivial, it is not clear if and how these states could be constructed. We will analyze this by looking at the thermo-majorization diagrams of states within the ϵ-balls.

4.2 Thermo-majorization

First, we will introduce a function that will be useful when the β-order of the eigenvalues are not preserved within the ϵ-ball.

For a d-dimensional state ρ that is diagonal in the energy eigenbasis, let $p = \{p_1, \dots, p_d\}$ be the vector containing the eigenvalues according to an ordered energy eigenbasis $E = \{E_1, \dots, E_d\}$. Then, we define the curve $c(p, E)$ which connects the points given by $\left\{\sum_{i=1}^k e^{-\beta E_i}/Z, \sum_{i=1}^k p_i\right\}$ with straight line segments. This curve depends on the order of the eigenvalues. If we have that the eigenvalues are β-ordered, such that $p_1 e^{\beta E_1} \geq \dots \geq p_d e^{\beta E_d}$, then this curve lines up with the thermo-majorization diagram of ρ.

Lemma 2. *Let ρ be a d-dimensional system, with $d \in \{\mathbb{N}, \infty\}$. Let $\{\hat{p}_i\}$ be the β-ordered eigenvalues of ρ, with $\{\hat{E}_i\}$ the corresponding energy levels. Let $\{p_i\}$ be the eigenvalues of ρ in an arbitrary order, with corresponding energy levels $\{E_i\}$. Then, $c(p, E) \leq c(\hat{p}, \hat{E})$.*

Proof. Since the order of p and E was arbitrary, there are two possible scenarios. It is possible that $p_1 e^{\beta E_1} \geq \dots \geq p_d e^{\beta E_d}$. In this case, we have that $\hat{p}_i = p_i$, and $\hat{E}_i = E_i$ for all i. Thus, the curves $c(p, E)$ and $c(\hat{p}, \hat{E})$ are the same, such that we clearly have that $c(p, E) \leq c(\hat{p}, \hat{E})$.

The other case is that $p_1 e^{\beta E_1} \geq \dots \geq p_d e^{\beta E_d}$ does not hold. This means, that we can find an index n such that $p_n e^{\beta E_n} < p_{n+1} e^{\beta E_{n+1}}$. We will look at this index more closely.

We define

$$\tilde{p}_i = \begin{cases} p_{n+1} & \text{if } i = n \\ p_n & \text{if } i = n+1 \\ p_i & \text{otherwise} \end{cases} \tag{166}$$

and

$$\tilde{E}_i = \begin{cases} E_{n+1} & \text{if } i = n \\ E_n & \text{if } i = n+1 \\ E_i & \text{otherwise.} \end{cases} \tag{167}$$

If we then compare $c(p, E)$ with $c(\tilde{p}, \tilde{E})$, we see that the curves are identical before the point $(\sum_{i=1}^{n-1} e^{-\beta E_i}/Z, \sum_{i=1}^{n-1} p_i)$ and after the point $(\sum_{i=1}^{n+1} e^{-\beta E_i}/Z, \sum_{i=1}^{n+1} p_i)$. Between those two points, the curves differ. Notice that both curves have one kink between the two points. We will compare these kinks with the straight line through $(\sum_{i=1}^{n-1} e^{-\beta E_i}/Z, \sum_{i=1}^{n-1} p_i)$ and $(\sum_{i=1}^{n+1} e^{-\beta E_i}/Z, \sum_{i=1}^{n+1} p_i)$.

To make this easier, we will redefine the origin to be located at $(\sum_{i=1}^{n-1} e^{-\beta E_i}/Z, \sum_{i=1}^{n-1} p_i)$. The straight line through the two points is then given by

$$\begin{aligned} y &= \frac{(p_n + p_{n+1})}{e^{-\beta E_n}/Z + e^{-\beta E_{n+1}}/Z} x & (168) \\ &= \frac{(p_n + p_{n+1})Z}{e^{-\beta E_n} + e^{-\beta E_{n+1}}} x. & (169) \end{aligned}$$

The kink of $c(p, E)$ is located at $(e^{-\beta E_n}/Z, p_n)$. The height difference between the straight line and the kink is given by

$$\begin{aligned} y - p_n &= \frac{(p_n + p_{n+1})Z}{e^{-\beta E_n} + e^{-\beta E_{n+1}}} e^{-\beta E_n}/Z - p_n & (170) \\ &= \frac{(p_n + p_{n+1})}{e^{-\beta E_n} + e^{-\beta E_{n+1}}} e^{-\beta E_n} - p_n \frac{e^{-\beta E_n} + e^{-\beta E_{n+1}}}{e^{-\beta E_n} + e^{-\beta E_{n+1}}} & (171) \\ &= \frac{e^{-\beta E_n}(p_n + p_{n+1}) - p_n(e^{-\beta E_n} + e^{-\beta E_{n+1}})}{e^{-\beta E_n} + e^{-\beta E_{n+1}}} & (172) \\ &= \frac{e^{-\beta E_n} p_{n+1} - e^{-\beta E_{n+1}} p_n}{e^{-\beta E_n} + e^{-\beta E_{n+1}}} & (173) \\ &= \frac{e^{\beta(E_n + E_n + 1)}(e^{-\beta E_n} p_{n+1} - e^{-\beta E_{n+1}} p_n)}{e^{\beta(E_n + E_n + 1)}(e^{-\beta E_n} + e^{-\beta E_{n+1}})} & (174) \\ &= \frac{e^{\beta E_{n+1}} p_{n+1} - e^{\beta E_n} p_n}{e^{\beta(E_n + E_n + 1)}(e^{-\beta E_n} + e^{-\beta E_{n+1}})} & (175) \\ &> 0. & (176) \end{aligned}$$

Thus, in the region of interest, $c(p, E)$ lies below the straight line. For $c(\tilde{p}, \tilde{E})$, which has it's kink located at $(e^{-\beta E_{n+1}}/Z, p_{n+1})$, we find the opposite.

$$
\begin{aligned}
y - p_{n+1} &= \frac{(p_n + p_{n+1})Z}{e^{-\beta E_n} + e^{-\beta E_{n+1}}} e^{-\beta E_{n+1}}/Z - p_{n+1} && (177)\\
&= \frac{(p_n + p_{n+1})}{e^{-\beta E_n} + e^{-\beta E_{n+1}}} e^{-\beta E_{n+1}} - p_{n+1} \frac{e^{-\beta E_n} + e^{-\beta E_{n+1}}}{e^{-\beta E_n} + e^{-\beta E_{n+1}}} && (178)\\
&= \frac{e^{-\beta E_{n+1}}(p_n + p_{n+1}) - p_{n+1}(e^{-\beta E_n} + e^{-\beta E_{n+1}})}{e^{-\beta E_n} + e^{-\beta E_{n+1}}} && (179)\\
&= \frac{e^{-\beta E_{n+1}} p_n - e^{-\beta E_n} p_{n+1}}{e^{-\beta E_n} + e^{-\beta E_{n+1}}} && (180)\\
&= \frac{e^{\beta(E_n + E_n + 1)}(e^{-\beta E_{n+1}} p_n - e^{-\beta E_n} p_{n+1})}{e^{\beta(E_n + E_n + 1)}(e^{-\beta E_n} + e^{-\beta E_{n+1}})} && (181)\\
&= \frac{e^{\beta E_n} p_n - e^{\beta E_{n+1}} p_{n+1}}{e^{\beta(E_n + E_n + 1)}(e^{-\beta E_n} + e^{-\beta E_{n+1}})} && (182)\\
&< 0, && (183)
\end{aligned}
$$

which means that in the region of interest, $c(\tilde{p}, \tilde{E})$ lies above the straight line, and therefore also above $c(p, E)$. Thus, if we perform a swap between neighbouring elements of p, such that after swapping the elements n and $n+1$ we have that $p_n e^{\beta E_n} \geq p_{n+1} e^{\beta E_{n+1}}$, then the height of the curve does not decrease anywhere, and increases at least somewhere.

Using this, we can define a sequence of distributions $\{q^n\}_{n=1}^m$ with corresponding energy levels $\{E^n\}_{n=1}^m$, with $m \in \{\mathbb{N}, \infty\}$. We define $q^1 = p$ and $E^1 = E$. Furthermore, we define q^{n+1} by performing a swap between neighbouring elements on q^n at index k, such that for q^{n+1} we have that $p_k e^{\beta E_k} \geq p_{k+1} e^{\beta E_{k+1}}$. E^{n+1} is defined by performing the same swap on E^n. Lastly, we pick m such that $q^m = \hat{p}$ and $E^m = \hat{E}$.

It may not be straightforward to see that $\hat{p}$ is always reached. Notice however, that $\hat{p}$ is the only vector for which no swaps can be made that increase the height of the curve. Thus, for as long as the β-order has not been reached, we can continue to perform swaps.

For this sequence, we have that $c(q^n, E^n) \leq c(q^{n+1}, E^{n+1})$. Thus, it follows that $c(p, E) = c(q^1, E^1) \leq \ldots \leq c(q^m, E^m) = c(\hat{p}, \hat{E})$. The β-order is the order for which the height of the curve is maximized. $\square$

This lemma will help us to prove some general constraints on thermo-majorization diagrams of states within ϵ-balls. These bounds will be useful when we are looking at steepest and flattest states, since the thermo-majorization curves of those states may have to reach the bounds. Otherwise, the thermo-majorization curves of other states might surpass the curves of the steepest and flattest states.

Theorem 7. *Let ρ be a d-dimensional system, with $d \in \{\mathbb{N}, \infty\}$, and let ρ' be a d-dimensional system within an ϵ-ball around ρ. Furthermore, let both ρ and ρ' be diagonal in the energy eigenbasis. Then, the height difference between the thermo-majorization curves of ρ and ρ' can never exceed ϵ. This is depicted in figure 12.*

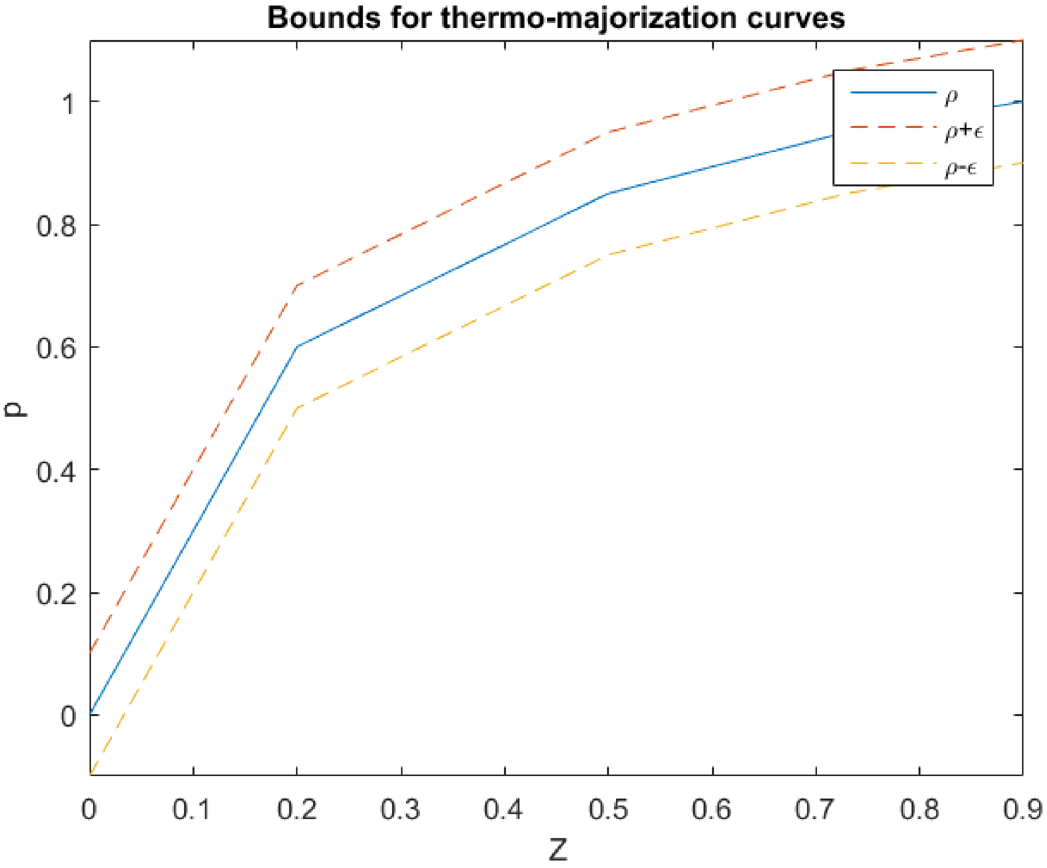

Figure 12: The thermo-majorization diagram of ρ together with the two bounds.

Proof. Let $p = \{p_i\}$ be the β-ordered eigenvalues of ρ with corresponding energy levels $E = \{E_i\}$, such that $p_1 e^{\beta E_1} \geq \ldots \geq p_d e^{\beta E_d}$. Let $p' = \{p'_i\}$ be the eigenvalues of ρ', in the same order as $\{p_i\}$. Notice that the energy levels E also correspond to the eigenvalues p'. Then, because ρ' is within an ϵ-ball around ρ, we have that

$$\frac{1}{2}\sum_{i=1}^{d} |p_i - p'_i| \leq \epsilon. \tag{184}$$

Furthermore, because both states are normalized, we have that

$$\sum_{i=1}^{d} (p_i - p'_i) = 0. \tag{185}$$

This means that

$$\sum_{i=1}^{d}(p_i - p_i') = \sum_{i:p_i>p_i'}(p_i - p_i') + \sum_{i:p_i<p_i'}(p_i - p_i') = 0 \tag{186}$$

And thus

$$\sum_{i:p_i>p_i'}(p_i - p_i') = -\sum_{i:p_i<p_i'}(p_i - p_i') \tag{187}$$

Combining these equations yields

$$\begin{align}
\frac{1}{2}\sum_{i=1}^{d}|p_i - p_i'| &= \frac{1}{2}\sum_{i:p_i>p_i'}(p_i - p_i') - \frac{1}{2}\sum_{i:p_i<p_i'}(p_i - p_i') \tag{188}\\
&= \sum_{i:p_i>p_i'}(p_i - p_i') \tag{189}\\
&= -\sum_{i:p_i<p_i'}(p_i - p_i') \leq \epsilon \tag{190}
\end{align}$$

Because p' and p are different, it might occur that the β-orders of p' and p are also different. We will first consider the case where both systems have the same β-order.

In this case, the kinks of both diagrams line up. This means that we only have to compare the height of the curves at these points. The height difference between the two curves is then given by

$$\begin{align}
\left|\sum_{i=1}^{k}p_i - \sum_{i=1}^{k}p_i'\right| &= \left|\sum_{i=1}^{k}(p_i - p_i')\right| \tag{191}\\
&= \left|\sum_{i\leq k:p_i>p_i'}(p_i - p_i') + \sum_{i\leq k:p_i<p_i'}(p_i - p_i')\right| \tag{192}\\
&= \left|\left|\sum_{i\leq k:p_i>p_i'}(p_i - p_i')\right| - \left|\sum_{i\leq k:p_i<p_i'}(p_i - p_i')\right|\right| \tag{193}\\
&\leq \max\left(\left|\sum_{i\leq k:p_i>p_i'}(p_i - p_i')\right|, \left|\sum_{i\leq k:p_i<p_i'}(p_i - p_i')\right|\right) \tag{194}\\
&\leq \epsilon. \tag{195}
\end{align}$$

Thus, without changing the β-order of the eigenvalues, the height difference between the thermo-majorization curves of ρ and ρ' cannot be larger than ϵ.

Next, we assume that the β-order of the eigenvalues is different for ρ and ρ'. We can use the curve defined earlier to show that the height difference between the two curves still cannot exceed ϵ.

To do this, we introduce the eigenvalues $q = \{q_i\}$, with corresponding energy levels $\hat{E} = \{\hat{E}_i\}$. First, we define q and $\hat{E}$ to be reordered versions of p' and E, such that q is β-ordered. Mathematically, this can be expressed as

$$q_i = p'_{n(i)} \tag{196}$$
$$\hat{E}_i = E_{n(i)}, \tag{197}$$

for all i, with $n : \{1, \ldots, d\} \to \{1, \ldots, d\}$ a bijection such that $p'_n(1)e^{\beta E_n(1)} \geq \ldots \geq p'_n(d)e^{\beta E_n(d)}$.

First of all, we have that the thermo-majorization curve of ρ is given by $c(p, E)$. As we showed earlier, without changing the order of the eigenvalues, the difference between the heights cannot exceed ϵ. Since the order of p' was assumed to be the same as the order of p, this yields

$$c(p', E) \geq c(p, E) - \epsilon. \tag{198}$$

Since q is the β-ordered version of p', it follows from lemma 2 that $c(q, \hat{E}) \geq c(p', E)$. This gives us that

$$c(q, \hat{E}) \geq c(p', E) \geq c(p, E) - \epsilon. \tag{199}$$

However, the thermo-majorization curve of ρ' is given by $c(q, \hat{E})$, and thus $c(p, E) - \epsilon$ is a lower bound for the thermo-majorization curve of any state within the ϵ-ball.

To prove that $c(p, E) + \epsilon$ is an upper bound for the thermo-majorization curve of ρ', we will need to define the eigenvalues $q^1 = \{q^1_i\}$ and $q^2 = \{q^2_i\}$, with corresponding energy levels $\hat{E} = \{\hat{E}_i\}$.

We define q^1 and $\hat{E}$ to be reordered versions of p and E respectively, such that they are in the β-order of ρ'. Mathematically, this can be expressed as

$$q^1_i = p_{n(i)} \tag{200}$$
$$\hat{E}_i = E_{n(i)}, \tag{201}$$

for all i, with $n : \{1, \dots, d\} \to \{1, \dots, d\}$ a bijection such that $p'_n(1) e^{\beta E_n(1)} \geq \dots \geq p'_n(d) e^{\beta E_n(d)}$.

We define q^2 by

$$q_i^2 = p'_{n(i)}, \tag{202}$$

with n the same bijection. Then, since q^1 is a reordered version of p, and p is β-ordered, we have that

$$c(q^1, \hat{E}) \leq c(p, E). \tag{203}$$

Next, we will compare $c(q^1, \hat{E})$ with $c(q^2, \hat{E})$. Because q^1 and q^2 are in the same order, comparing the kinks of the curves is sufficient. Notice that both q^1 and q^2 are normalized. We also have that

$$\frac{1}{2} \sum_{i=1}^{d} \left| q_i^1 - q_i^2 \right| = \frac{1}{2} \sum_{i=1}^{d} |p_i - p'_i| \leq \epsilon. \tag{204}$$

Therefore, equations 184 through 195 hold for q^1 and q^2. Thus the height difference between $c(q^1, \hat{E})$ and $c(q^2, \hat{E})$ cannot exceed ϵ. This yields

$$\begin{aligned} c(q^2, \hat{E}) &\leq c(q^1, \hat{E}) + \epsilon & (205) \\ &\leq c(p, E) + \epsilon. & (206) \end{aligned}$$

Because the thermo-majorization curve of ρ' is given by $c(q^2, \hat{E})$, we find that $c(p, E) + \epsilon$ is an upper bound.

The conclusion follows: whether or not the β orders of the eigenvalues are different for ρ and ρ', the height difference between the thermo-majorization curves of ρ and ρ' cannot exceed ϵ. □

This theorem gives us some bounds for the thermo-majorization curves of the states within the ϵ-ball. Notice however, that the bounds cannot always be reached; at some point, one of the bounds becomes negative. At another point, the other bound becomes larger than 1. Because the eigenvalues form a normalized probability distribution, these bounds clearly cannot be reached there.

Nevertheless, when looking at the steepest and flattest states, we will try to reach the bound for as long as possible.

4.3 The steepest state

We start by analyzing the steepest state. We will do this by looking at thermo-majorization, while heavily restricting the size of the ϵ-ball. Notice that, because we are looking at thermo-majorization, if we cannot find a steepest state for some ρ or some ϵ, this does not mean that there exists no steepest state. Maybe with the use of a catalyst, a steepest state can be found. This is not what we will be looking at, however.

Let ρ be a d-dimensional system, with β-ordered eigenvalues p_i and corresponding energy levels E_i. The steepest state of ρ has slightly modified eigenvalues, such that it is still within an ϵ-ball around ρ.

When changing the eigenvalues, we can also change the β-order. This is, however, something we want to avoid. If, by changing the eigenvalues, we change the β-order, we effectively waste a small portion of ϵ. This would likely cause the resulting state to not be a steepest state. Thus, we will keep the order of the eigenvalues the same for ρ and the steepest state.

We will first bound ϵ such that we only have to modify two eigenvalues. When modifying more than two eigenvalues, it is no longer clear which ones have to be modified. On one hand, we have to maximize the region where the thermo-majorization curve is equal to 1. On the other hand, we should avoid changing the β-order. Because it is unclear if these things can be achieved simultaneously, we will avoid changing more than two eigenvalues. The resulting bound on ϵ is given by

$$\epsilon \leq \min_{i:p_i>0} (p_i) . \tag{207}$$

Now that we only have to modify two eigenvalues, we need to find out which eigenvalues we have to alter. Clearly, since we are not changing the β-order, we have to modify the first eigenvalue, and the last nonzero eigenvalue. This does not always exactly determine which eigenvalue we have to change, however, as it can occur that $p_1 e^{\beta E_1} = \ldots = p_m e^{\beta E_m}$ for the first m eigenvalues, or that $p_n e^{\beta E_n} = \ldots = p_k e^{\beta E_k}$, where p_k is the last nonzero eigenvalue.

In these cases, we will want to modify the smallest eigenvalues; it is for these eigenvalues that our adjustment will have the largest impact on the slope. Thus, we will not only define p_i to be β-ordered. We also require that $p_1 = \min_{i \leq m}(p_i)$, and that $p_k = \min_{n \leq i \leq k}(p_i)$.

This further restricts the states for which we can find a steepest state. If ρ is equal to a sharp state, a state for which we have that $p_1 e^{\beta E_1} = \ldots = p_m e^{\beta E_m}$ and $p_i = 0$ for all $i > m$, it is generally not the case that the highest energy eigenstate with a nonzero eigenvalue is degenerate. This is, however, what we require: we want the smallest eigenvalue to be both the first and the last eigenvalue. For this reason, we will exclude sharp states from our method.

We already posed one bound for ϵ so far. Now that we know which eigenvalues we will modify, we can determine more bounds for ϵ. These bounds combined will define when we are able to construct the steepest state.

The second boundary arises when making sure that the slope of the first eigenvalue of the steepest state is the steepest slope we could possibly create. We will restrict ϵ such that $(p_1 + \epsilon)\, e^{\beta E_1} \geq (p_i + \epsilon)\, e^{\beta E_i}$ for all $1 < i \leq n$. Notice that this is true by default if $E_i = E_1$. If $E_i \neq E_1$, We have that

$$\epsilon \left(e^{\beta E_1} - e^{\beta E_i}\right) \geq p_i e^{\beta E_i} - p_1 e^{\beta E_1}. \tag{208}$$

Depending on the sign of $\left(e^{\beta E_1} - e^{\beta E_i}\right)$, this is equivalent with either

$$\epsilon \geq \frac{p_i e^{\beta E_i} - p_1 e^{\beta E_1}}{e^{\beta E_1} - e^{\beta E_i}}, \tag{209}$$

or

$$\epsilon \leq \frac{p_i e^{\beta E_i} - p_1 e^{\beta E_1}}{e^{\beta E_1} - e^{\beta E_i}}. \tag{210}$$

Notice that by assumption, $p_1 e^{\beta E_1} \geq p_i e^{\beta E_i}$, and thus in the former case, we require ϵ to be larger than some negative number, which it is by default. Restrictions do arise when $E_i > E_1$. Thus, we have that

$$\epsilon \leq \min_{i \neq 1 : E_i > E_1} \left(\frac{p_1 e^{\beta E_1} - p_i e^{\beta E_i}}{e^{\beta E_i} - e^{\beta E_1}} \right). \tag{211}$$

The third and last restriction appears when we make sure that the slope of the last nonzero eigenvalue of the steepest state is the flattest slope we could possibly create by changing nonzero eigenvalues.

Recall that k was defined as the largest index for which $p_k e^{\beta E_k}$ is minimized while also $p_k > 0$. We then restrict ϵ such that $(p_k - \epsilon)\, e^{\beta E_k} \leq (p_i - \epsilon)\, e^{\beta E_i}$. Notice that this is automatically true if $E_i = E_k$. If $E_i \neq E_k$, We have that

$$(p_k - \epsilon)\, e^{\beta E_k} \leq (p_i - \epsilon)\, e^{\beta E_i}. \tag{212}$$

Moving all terms with ϵ to the left hand side yields

$$\epsilon\left(e^{\beta E_i}-e^{\beta E_k}\right)\leq p_i e^{\beta E_i}-p_k e^{\beta E_k}. \tag{213}$$

Much like before, this gives us two possible restrictions, depending on the sign of $\left(e^{\beta E_i}-e^{\beta E_k}\right)$. We have that either

$$\epsilon\leq\frac{p_i e^{\beta E_i}-p_k e^{\beta E_k}}{e^{\beta E_i}-e^{\beta E_k}}, \tag{214}$$

or

$$\epsilon\geq\frac{p_i e^{\beta E_i}-p_k e^{\beta E_k}}{e^{\beta E_i}-e^{\beta E_k}}. \tag{215}$$

Because $\left(p_i e^{\beta E_i}-p_k e^{\beta E_k}\right)$ is always positive, the latter case reduces to requiring ϵ to be positive, which it is by default. The bound for ϵ becomes

$$\epsilon\leq\min_{i\neq k:p_i>0,E_i>E_k}\left(\frac{p_i e^{\beta E_i}-p_k e^{\beta E_k}}{e^{\beta E_i}-e^{\beta E_k}}\right). \tag{216}$$

For these ϵ, we define the eigenvalues of the steepest state of ρ such that

$$\hat{p}_i=\begin{cases}p_i+\epsilon & \text{if } i=1\\ p_i-\epsilon & \text{if } i=k\\ p_i & \text{otherwise.}\end{cases} \tag{217}$$

We will now show that when these restrictions are met, this state is the steepest state within the ϵ-ball.

Theorem 8. *Let ρ be a state that is diagonal in the energy eigenbasis. If ϵ satisfies*

$$\epsilon\leq\min\left\{\min_{i:p_i>0}(p_i),\min_{i:E_i>E_1}\left(\frac{p_1 e^{\beta E_1}-p_i e^{\beta E_i}}{e^{\beta E_i}-e^{\beta E_1}}\right),\min_{i:p_i>0,E_i>E_k}\left(\frac{p_i e^{\beta E_i}-p_k e^{\beta E_k}}{e^{\beta E_i}-e^{\beta E_k}}\right)\right\}, \tag{218}$$

Then there exists a steepest state $\rho^{\epsilon}_{steep}\in B^{\epsilon}(\rho)$ that thermo-majorizes all other states within the ball, with eigenvalues given by equation 217.

Proof. We will divide the thermo-majorization curve up in multiple regions, and show for each region that no other state within the ϵ-ball has a thermo-majorization curve that can surpass it. This is depicted in figure 13.

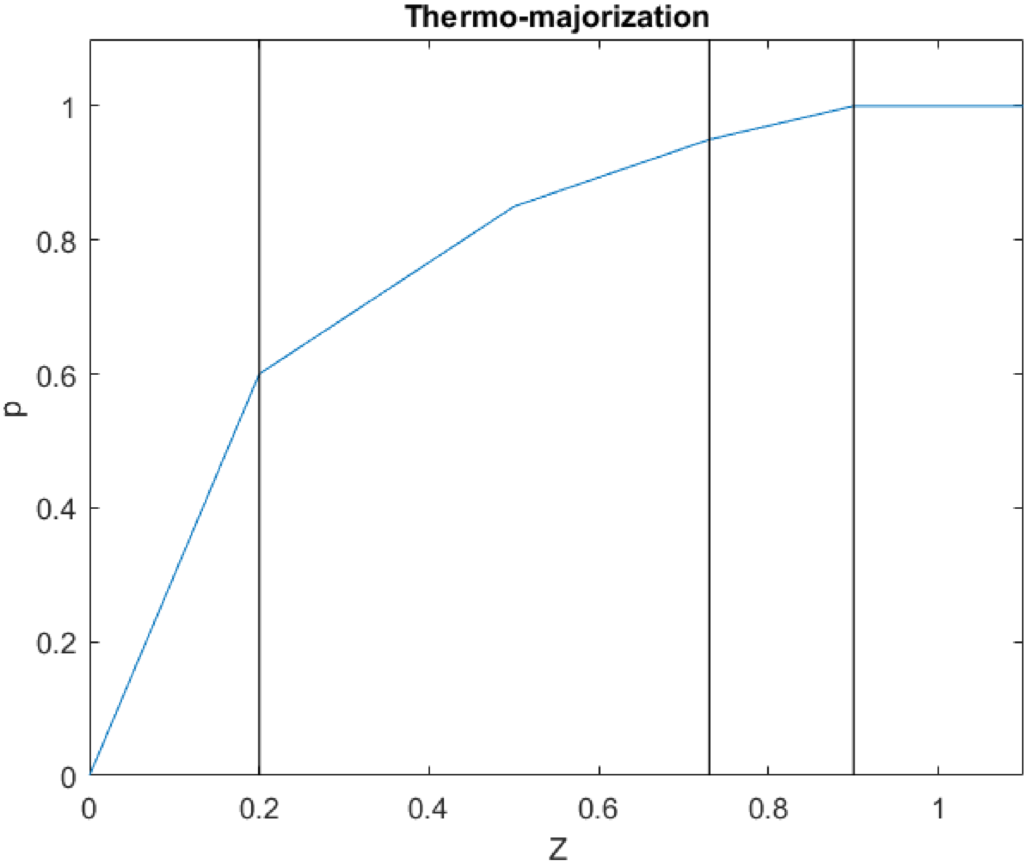

Figure 13: The thermo-majorization diagram divided up in four regions.

The first region is the region to the left of $(e^{-\beta E_1}, \hat{p}_1)$. For this region, it is clearly impossible for any other state to be steeper than the steepest state; we restricted ϵ such that this is the case. Notice that the bound given by theorem 7 is exactly reached at the edge of this region: $(e^{-\beta E_1}, \hat{p}_1)$ lies exactly ϵ above $(e^{-\beta E_1}, p_1)$.

The second region is the region between $(e^{-\beta E_1}, \hat{p}_1)$ and $(\sum_{i=1}^{k-1} e^{-\beta E_i}, \sum_{i=1}^{k-1} \hat{p}_i)$. For this region, the thermo-majorization diagram of the steepest state lies exactly ϵ above the thermo-majorization diagram of ρ. As a result of theorem 7, it is impossible to surpass this while staying within the ϵ-ball.

The third region is the region between $(\sum_{i=1}^{k-1} e^{-\beta E_i}, \sum_{i=1}^{k-1} \hat{p}_i)$ and $(\sum_{i=1}^{k} e^{-\beta E_i}, 1)$. Since the thermo-majorization curve of the steepest state reaches 1 at the edge of this region, it is not possible to surpass it in this region without having a flatter slope than the curve of the steepest state has. Our restrictions to ϵ ensure that this is impossible, however. Thus, in this region, the thermo-majorization curve of the steepest state cannot be surpassed.

The last region is the region to the right of $(\sum_{i=1}^{k} e^{-\beta E_i}, 1)$. Clearly, because the states are normalized, it is impossible for any state to have a thermo-majorization curve that surpasses 1.

Since for all regions, the thermo-majorization curve of the steepest state cannot be surpassed, this state thermo-majorizes all other states within the ϵ-ball. $\square$

We will give an example to illustrate this further. In this example we will also show that when the restrictions to ϵ are not met, the steepest state as we defined it does not always thermo-majorize all other states within the ϵ-ball.

Example 4.1. Let ρ be a 5-dimensional quantum system with eigenvalues given by $\{0.25, 0.1, 0.3, 0.2, 0.15\}$. For the sake of simplicity, we will define the values of $e^{\beta E_i}$ rather than defining the energy levels themselves. Let $e^{\beta E_i}$ be given by $\{5, 10, 3, 2, 1\}$. Notice that the eigenvalues are β-ordered.

First, we note that this state is not a sharp state. Thus, we can proceed to find the bounds for ϵ given in theorem 8. We have that

$$\epsilon \leq \min\left\{ \min_{i:p_i>0}(p_i), \min_{i:E_i>E_1}\left(\frac{p_1 e^{\beta E_1} - p_i e^{\beta E_i}}{e^{\beta E_i} - e^{\beta E_1}}\right), \min_{i:p_i>0, E_i>E_k}\left(\frac{p_i e^{\beta E_i} - p_k e^{\beta E_k}}{e^{\beta E_i} - e^{\beta E_k}}\right)\right\} \tag{219}$$

$$= \min\{0.1, 0.05, 0.0944\} \tag{220}$$

$$= 0.05. \tag{221}$$

We will first choose $\epsilon = 0.05$. The eigenvalues of ρ^{ϵ}_{steep} are then given by $\{0.3, 0.1, 0.3, 0.2, 0.1\}$. We give the thermo-majorization diagram of ρ and ρ^{ϵ}_{steep} in figure 14.

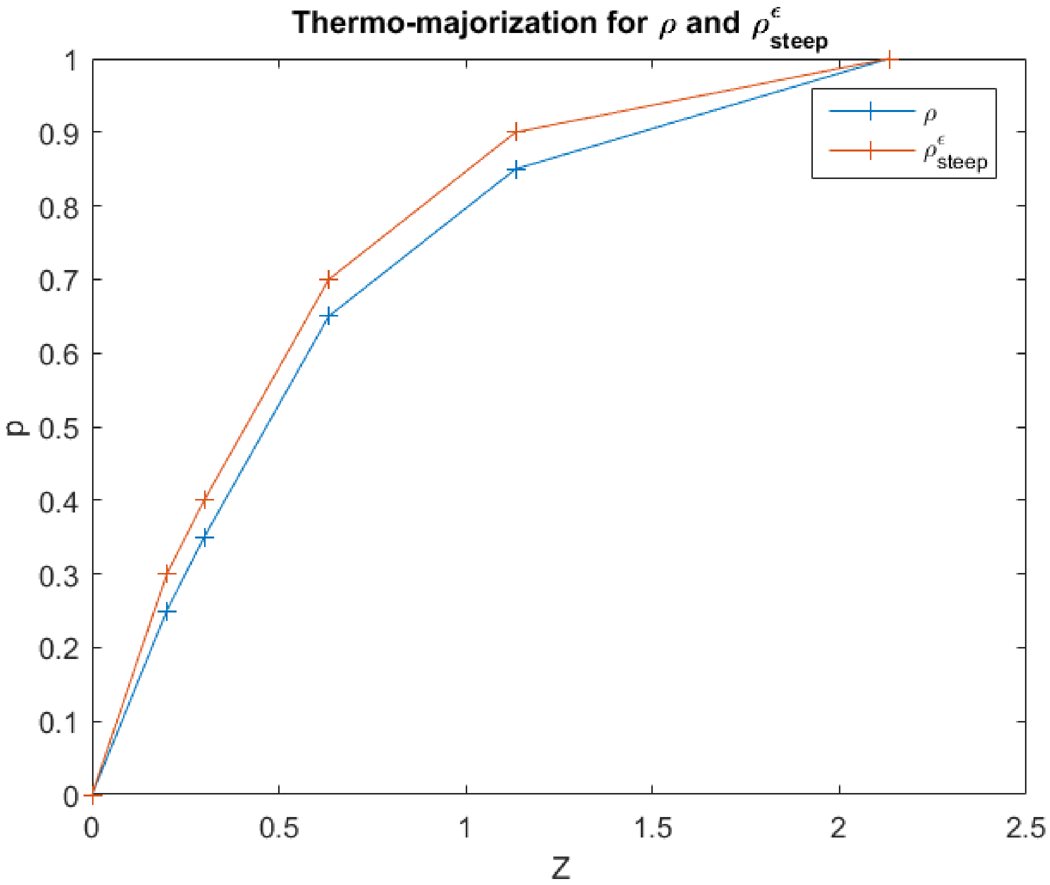

Figure 14: The thermo-majorization diagram of ρ and ρ^{ϵ}_{steep}. The kinks of both curves have been marked to them easier to see.

Next, we will consider what happens if $\epsilon > 0.05$. To do this, we choose $\epsilon = 0.1$. If we then follow the same procedure to create a steep state, a state that thermo-majorizes ρ, but is not necessarily the steepest state, we would obtain the eigenvalues $\{0.35, 0.1, 0.3, 0.2, 0.05\}$.

Notice that the bound $\epsilon \leq \min_{i:E_i>E_1}\left(\frac{p_1 e^{\beta E_1} - p_i e^{\beta E_i}}{e^{\beta E_i} - e^{\beta E_1}}\right)$ is one of the bounds that is being violated in this scenario. Thus, we can probably find a state that is not thermo-majorized by our steep state by looking at this bound more closely

In this case, this bound follows from the second eigenvalue, such that

$$\epsilon > \frac{p_1 e^{\beta E_1} - p_2 e^{\beta E_2}}{e^{\beta E_2} - e^{\beta E_1}}. \tag{222}$$

Thus, by increasing the second eigenvalue instead we obtain a new state ρ' with eigenvalues $\{0.25, 0.2, 0.3, 0.2, 0.05\}$. In figure 15, the thermo-majorization diagram of ρ, ρ^{ϵ}_{steep} and ρ' is depicted.

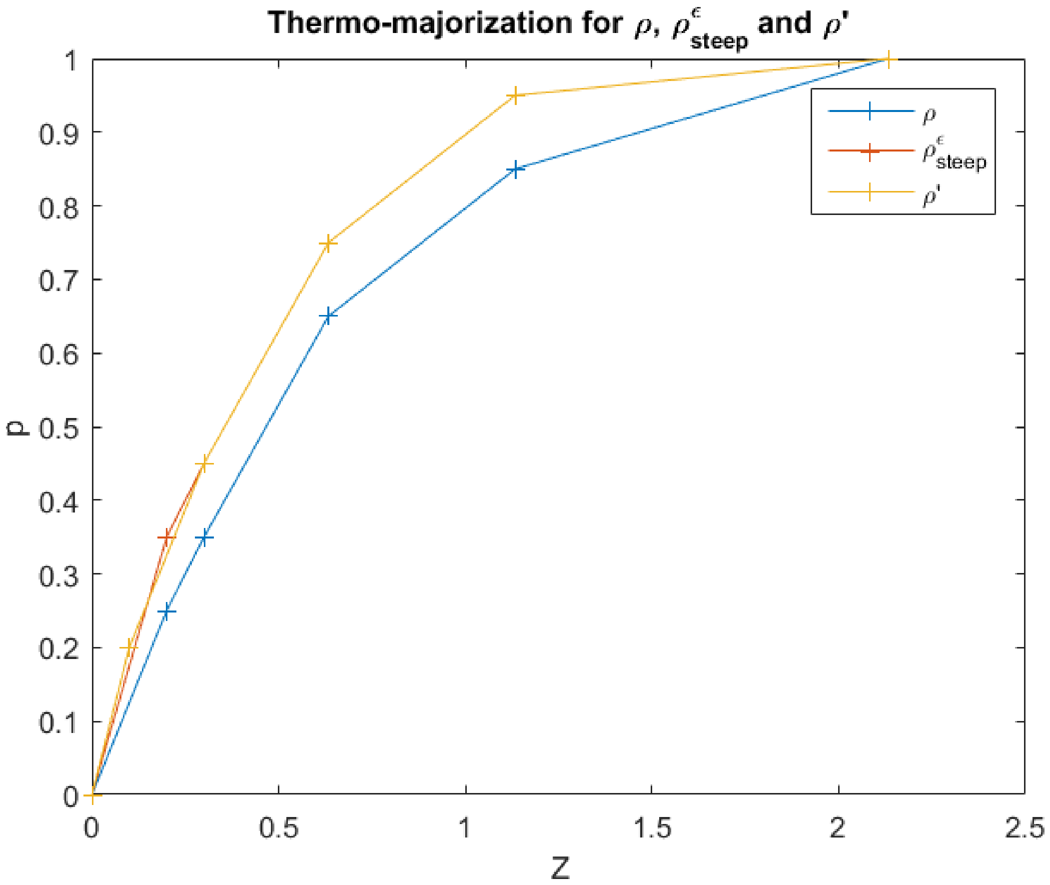

Figure 15: The thermo-majorization diagram of ρ, ρ^{ϵ}_{steep} and ρ'. The kinks of both curves have been marked to them easier to see. Here, ρ^{ϵ}_{steep} denotes the steep state that we constructed, which thermo-majorizes ρ, but not necessarily all other states that are ϵ-close to ρ.

It is clear that for the most part, ρ^{ϵ}_{steep} and ρ' have the same thermo-majorization curve. However, the first few line segments differ. A more zoomed in thermo-majorization diagram is given in figure 16.

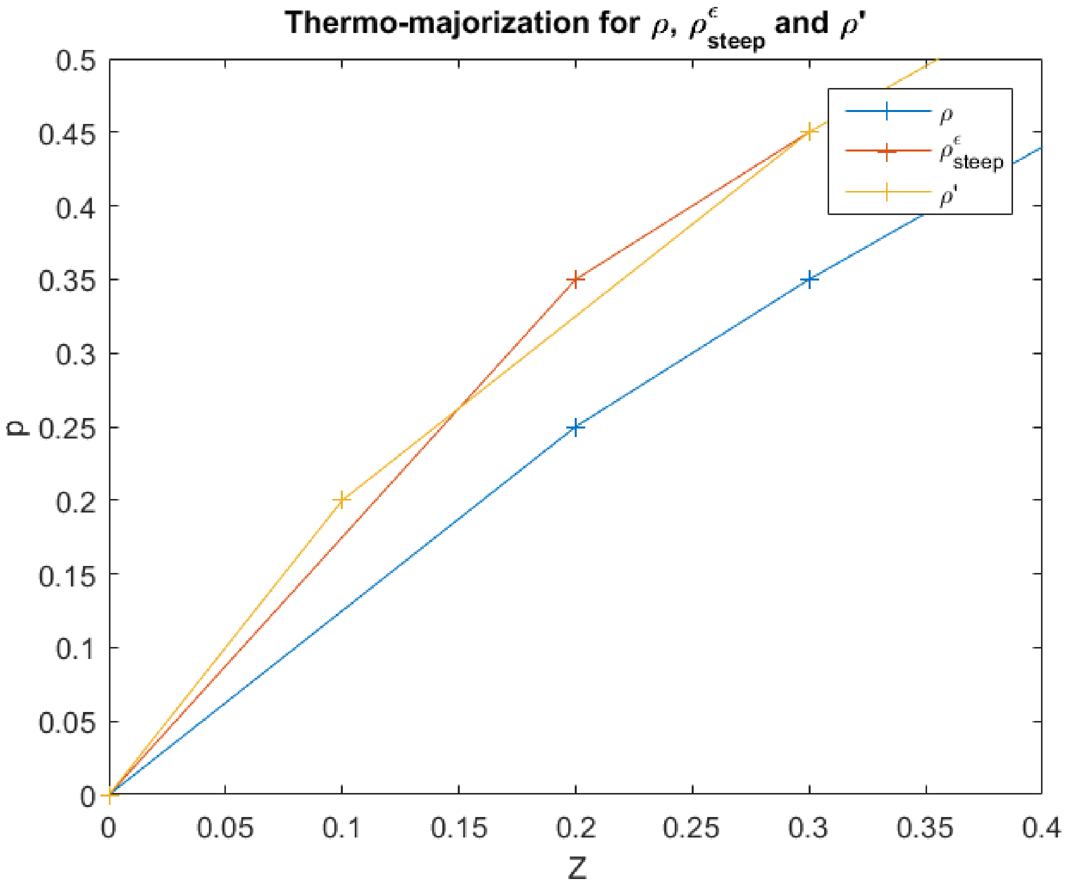

Figure 16: The thermo-majorization diagram of ρ, ρ^{ϵ}_{steep} and ρ'. The kinks of both curves have been marked to them easier to see. Clearly, ρ^{ϵ}_{steep} and ρ' are incomparable.

Clearly, the thermo-majorization curves of ρ^{ϵ}_{steep} and ρ' intersect. Thus, the states are incomparable. This means that the steep state cannot be transformed into all other states within the ϵ-ball around ρ by thermal operations. This does not, however, exclude the possibility that there exists a steepest state. Also, it might be the case that ρ^{ϵ}_{steep} can be transformed to all other states when catalysts come into play. We will not answer these questions in this work, however.

4.4 The flattest state

In this section, we will analyze the flattest state. We will first provide a way to construct it, and after that we give an example.

Theorem 9. *Unlike the steepest state, for any ϵ-ball we can find a state that is thermo-majorized by all states within the ball.*

Proof. Let ρ be an d-dimensional system and let p_i be the β-ordered eigenvalues of ρ with corresponding energy levels E_i. We will attempt to find ρ_{flat}, the flattest state of ρ with eigenvalues $\hat{p}_i$.

We will consider two cases. If ϵ is large enough, such that

$$\frac{1}{2}\sum_{i=1}^{n}\left|p_i - \frac{e^{-\beta E_i}}{\sum_{j=1}^{n} e^{-\beta E_j}}\right| \leq \epsilon, \tag{223}$$

then the flattest state is equal to the thermal state, which is thermo-majorized by all other states. Thus, for large ϵ, the flattest state clearly exists.

if ϵ is not that large, it is not as straightforward to see that the flattest state exists. However, we will present a way to construct this state, and prove that this state is thermo-majorized by all other states within the ϵ-ball.

Assume that ϵ is large enough that we cannot reach the thermal state. Even though we can change the eigenvalues almost freely, we will avoid changing the β-order of the eigenvalues. We do this, because changing the β-order effectively wastes small portions of ϵ, resulting in smaller changes with respect to the thermo-majorization curve. We will first try to lower the first M_1 eigenvalues, such that $\hat{p}_1 e^{\beta E_1} = \hat{p}_2 e^{\beta E_2} = \ldots = \hat{p}_{M_1} e^{\beta E_{M_1}}$. These eigenvalues satisfy

$$\hat{p}_i e^{\beta E_i} = (p_i - \epsilon_i)\, e^{\beta E_i} \geq p_{M_1+1} e^{\beta E_{M_1+1}}, \tag{224}$$

from which it follows that

$$\epsilon_i \leq \frac{p_i e^{\beta E_i} - p_{M_1+1} e^{\beta E_{M_1+1}}}{e^{\beta E_i}}. \tag{225}$$

Using this information, we can determine M_1 such that:

$$\epsilon = \sum_{i=1}^{M_1} \epsilon_i \leq \sum_{i=1}^{M_1} \left(\frac{p_i e^{\beta E_i} - p_{M_1+1} e^{\beta E_{M_1+1}}}{e^{\beta E_i}} \right), \tag{226}$$

while making sure that this does not hold for $M_1 - 1$, such that

$$\epsilon > \sum_{i=1}^{M_1-1} \left(\frac{p_i e^{\beta E_i} - p_{M_1} e^{\beta E_{M_1}}}{e^{\beta E_i}} \right). \tag{227}$$

This value will tell us how many eigenvalues we have to change in order to fully use up ϵ. In a similar way, we can also determine $M_2 \in \mathbb{N}$, which tells us how many eigenvalues we have to increase. For M_2 we have that

$$\hat{p}_i e^{\beta E_i} = (p_i + \epsilon_i)\, e^{\beta E_i} \leq p_{M_2-1} e^{\beta E_{M_2-1}}, \tag{228}$$

from which it follows that

$$\epsilon_i \leq \frac{p_{M_2-1} e^{\beta E_{M_2-1}} - p_i e^{\beta E_i}}{e^{\beta E_i}}. \tag{229}$$

Using this information, we can determine M_2 such that

$$\epsilon = \sum_{i=M_2}^{n} \epsilon_i \leq \sum_{i=M_2}^{n} \left(\frac{p_{M_2-1} e^{\beta E_{M_2-1}} - p_i e^{\beta E_i}}{e^{\beta E_i}} \right), \tag{230}$$

while making sure that this does not hold for $M_2 + 1$, such that

$$\epsilon > \sum_{i=M_2+1}^{n} \left(\frac{p_{M_2} e^{\beta E_{M_2}} - p_i e^{\beta E_i}}{e^{\beta E_i}} \right). \tag{231}$$

Notice that it might happen that the eigenvalue with which we calculated these bounds changes as well. This is, however, not a problem; if we were to change the $(M_1 + 1)$-th and the $(M2 - 1)$-th eigenvalues further than would be allowed without changing the β-order, then it is possible to reach the thermal state. That means that our assumption about ϵ is violated, which yields a contradiction.

We can now determine the eigenvalues of the flattest state. Consider the first M_1 eigenvalues. For these eigenvalues we have that

$$\hat{p}_1 e^{\beta E_1} = \hat{p}_2 e^{\beta E_2} = \ldots = \hat{p}_{M_1} e^{\beta E_{M_1}} = c_1, \tag{232}$$

where c_1 is an unknown constant. Furthermore, we know that

$$\hat{p}_i = p_i - \epsilon_i. \tag{233}$$

Summing over the first M_1 eigenvalues of the flattest state gives us that

$$\sum_{i=1}^{M_1} p_i - \epsilon_i = \sum_{i=1}^{M_1} \hat{p}_i \tag{234}$$

$$= \sum_{i=1}^{M_1} \hat{p}_i e^{\beta E_i} e^{-\beta E_i} \tag{235}$$

$$= \sum_{i=1}^{M_1} c_1 e^{-\beta E_i} \tag{236}$$

$$= c_1 \sum_{i=1}^{M_1} e^{-\beta E_i} \tag{237}$$

and

$$\sum_{i=1}^{M_1} p_i - \epsilon_i = \left(\sum_{i=1}^{M_1} p_i \right) - \epsilon. \tag{238}$$

Combining these results yields

$$c_1 = \frac{c_1 \sum_{i=1}^{M_1} e^{-\beta E_i}}{\sum_{i=1}^{M_1} e^{-\beta E_i}} \tag{239}$$

$$= \frac{\left(\sum_{i=1}^{M_1} p_i \right) - \epsilon}{\sum_{i=1}^{M_1} e^{-\beta E_i}}. \tag{240}$$

This gives us the first M_1 eigenvalues. We have that

$$\hat{p}_i = e^{-\beta E_i} \frac{\left(\sum_{i=1}^{M_1} p_i \right) - \epsilon}{\sum_{i=1}^{M_1} e^{-\beta E_i}}. \tag{241}$$

We can determine the last $n+1-M2$ eigenvalues in a similar way. For these eigenvalues we find that

$$\hat{p}_i = e^{-\beta E_i} \frac{\epsilon + \sum_{i=M_2}^{n} p_i}{\sum_{i=M_2}^{n} e^{-\beta E_i}}. \tag{242}$$

All other eigenvalues are left unchanged. Thus, the flattest state is given by

$$\hat{p}_i = \begin{cases} e^{-\beta E_i} \frac{\left(\sum_{i=1}^{M_1} p_i \right) - \epsilon}{\sum_{i=1}^{M_1} e^{-\beta E_i}} & \text{if } i \leq M_1 \\ e^{-\beta E_i} \frac{\epsilon + \sum_{i=M_2}^{n} p_i}{\sum_{i=M_2}^{n} e^{-\beta E_i}} & \text{if } i \geq M_2 \\ p_i & \text{otherwise.} \end{cases} \tag{243}$$

Now we just need to show that this state is thermo-majorized by all other states within the ϵ-ball. To do this, we will divide the thermo-majorization curve up into three different regions, similar to what we did earlier. These regions are depicted in figure 17.

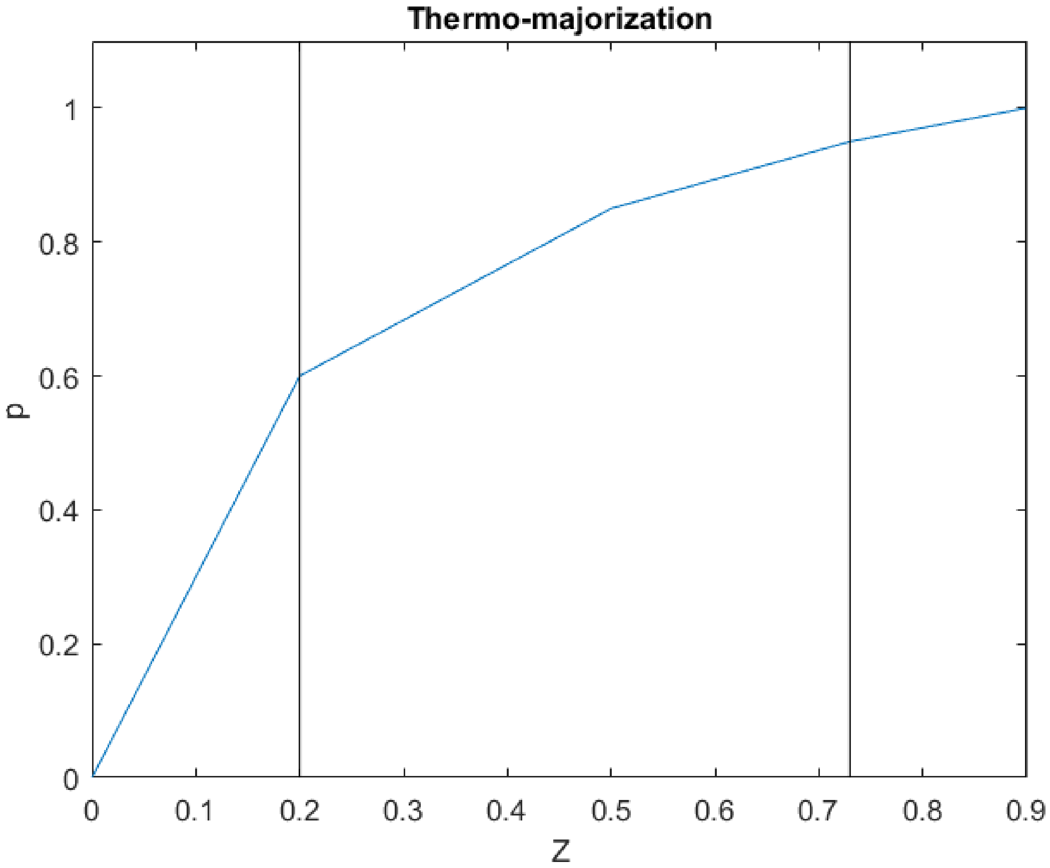

Figure 17: The thermo-majorization diagram of the flattest state divided up into three regions.

First, consider the region to the left of $(\sum_{i=1}^{M_1} e^{-\beta E_i}, \sum_{i=1}^{M_1} \hat{p}_i)$. For this region, the thermo-majorization curve of the flattest state is a straight line. The only way a state could possibly have a curve that lies below it, is when that curve lies below the thermo-majorization curve of the flattest state at $(\sum_{i=1}^{M_1} e^{-\beta E_i}, \sum_{i=1}^{M_1} \hat{p}_i)$. Notice that this is true because thermo-majorization curves are concave. However, by theorem 7 this is impossible, since at that location the thermo-majorization curve of the flattest state lies exactly ϵ below the curve of the initial state.

Next, we consider the region between $(\sum_{i=1}^{M_1} e^{-\beta E_i}, \sum_{i=1}^{M_1} \hat{p}_i)$ and $(\sum_{i=1}^{M_2} e^{-\beta E_i}, \sum_{i=1}^{M_2} \hat{p}_i)$. For this entire region, the curve of the flattest state lies ϵ below the curve of the initial state. For the same reason as before, no state can have a curve that lies lower than the curve of the flattest state in this region.

For the last region, the region to the right of $(\sum_{i=1}^{M_2} e^{-\beta E_i}, \sum_{i=1}^{M_2} \hat{p}_i)$, the thermo-majorization curve of the flattest state is, again, a straight line. For a state to have a curve that lies below it, this curve needs to lie below the point $(\sum_{i=1}^{M_2} e^{-\beta E_i}, \sum_{i=1}^{M_2} \hat{p}_i)$, again because thermo-majorization curves are concave. By theorem 7 this is impossible.

Since the thermo-majorization diagram of the flattest state cannot surpass the diagram of any other state at any point, the flattest state is thermo-majorized by all other states. This completes the proof, as we have successfully found a state that is thermo-majorized by all other states within an ϵ-ball, for any value of ϵ. $\square$

We will give an example to illustrate this.

Example 4.2. Let ρ be a 5-dimensional quantum system with eigenvalues given by $\{0.25, 0.1, 0.3, 0.2, 0.15\}$. For the sake of simplicity, we will define the values of $e^{\beta E_i}$ rather than defining the energy levels themselves. Let $e^{\beta E_i}$ be given by $\{5, 10, 3, 2, 1\}$. Notice that the eigenvalues are β-ordered. Furthermore, let $\epsilon = 0.15$.

We will first determine the values of M_1 and M_2. We find that $M_1 = 3$ and $M_2 = 5$. Thus, we need to decrease three different eigenvalues, but we only have to increase a single eigenvalue.

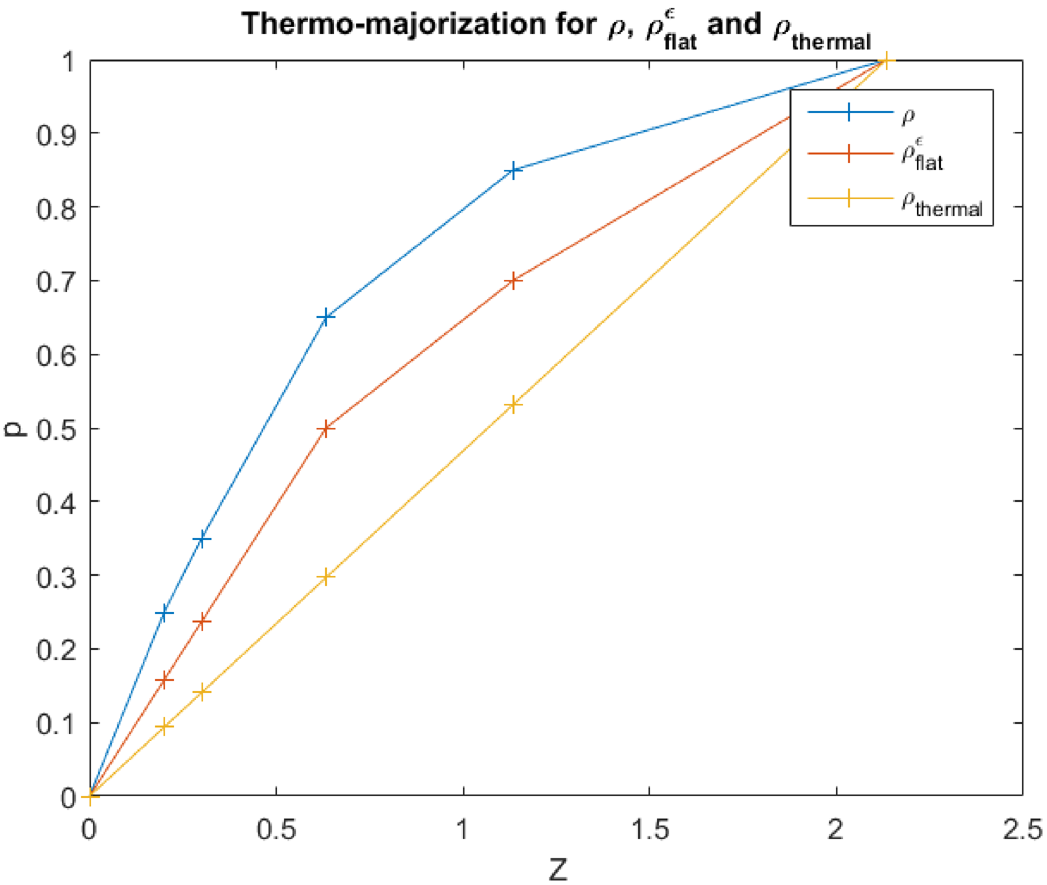

Figure 18: The thermo-majorization diagram of ρ^{ϵ}_{flat} and $\rho_{thermal}$.

The resulting eigenvalues are then given by $\{0.1579, 0.0789, 0.2632, 0.2, 0.3\}$. The thermo-majorization diagram of ρ, ρ^{ϵ}_{flat} and $\rho_{thermal}$ is depicted in figure 18.

With this we end the discussion on Rényi divergences. We have successfully found a region for ϵ for which the inequality $D^{\epsilon}_{\alpha}(\rho||\tau) \geq D^{\epsilon}_{\alpha}(\sigma||\tau)$ for all $\alpha \in \mathbb{R}$ is equivalent with a transition from ρ^{ϵ}_{steep} to σ^{ϵ}_{flat} being possible. Unfortunately, this region is quite small, depending on the states at question. Especially for states of infinite dimension, where generally the energy levels are unbounded, this becomes a problem. Thus, it is desirable to find an extension, or to look further at the impact of a catalyst on this steepest state.

Another option would be to define new smoothed divergences. In more recent work, we defined new divergences by

$$\hat{D}^{\epsilon}_{\alpha}(\rho||\tau) = \begin{cases} D_{\alpha}(\rho^{\epsilon}_{flat}||\tau) & \text{if } \alpha < 0 \\ D_{\alpha}(\rho^{\epsilon}_{steep}||\tau) & \text{if } 0 \leq \alpha \leq 1 \\ D_{\alpha}(\rho^{\epsilon}_{flat}||\tau) & \text{if } \alpha > 1, \end{cases} \tag{244}$$

where ρ_{flat} is the flattest state, and ρ_{steep} is a steep state. We construct this steep state by cutting the smallest β-ordered eigenvalues of ρ, and adding ϵ to the largest β-ordered eigenvalue. In that work, we showed that these new divergences also satisfy the asymptotic equipartition property, such that for all $\alpha \in \mathbb{R}$ and for any $0 < \epsilon < 1$,

$$\lim_{n\to\infty} \frac{1}{n}\hat{D}^{\epsilon}_{\alpha}(\rho^{\otimes n}||\tau^{\otimes n}) = D(\rho||\tau). \tag{245}$$

5 Conclusion

A simple way to describe how a quantum system evolves under energy-preserving unitaries while interacting with thermal reservoirs, has been formulated in the framework of thermal operations. By allowing the use of ancillary states as catalysts in these processes, a more general set of thermodynamical operations is obtained, called catalytic thermal operations. Despite the conceptual simplicity of these types of thermodynamical operations, much is still unknown about their mathematical structures. In this work, we studied these mathematical structures, in an attempt to better understand how these operations describe quantum thermodynamics.

One of the phenomena that we studied, is super-activation. We found that, when the Hamiltonians are trivial, qubits cannot super-activate each other. Furthermore, we found a way to construct examples of super-activation, both for trivial and nontrivial Hamiltonians. We also investigated a special instance of super-activation that we call self-activation. We found necessary conditions for self-activation to occur. These conditions show that self-activation can only happen in one direction.

We have also studied Rényi divergences. We have found that for certain ϵ-balls, the smoothed Rényi divergences decrease from a state ρ to a state σ if and only if a transition from the steepest state of ρ to the flattest state of σ is possible. These restrictions for ϵ arise because the steepest state does not always seem to exist. In contrary, we found that the flattest state can always be found.

For further research, it would be very useful if we could find sufficient conditions for self-activation to occur. Self-activation seems to be a rare phenomenon, and despite the fact that the necessary conditions that we found can be used to narrow down the set of states that can self-activate, it can be difficult to find examples. Having examples of this phenomenon would be useful to discover more about its properties. It would also be interesting if we could say something about the number of copies that is required to make the transition possible.

In this work we focused mainly on thermal operations. Catalysts can have a huge impact on the possibilities, however. It would be interesting to know more about their interaction with super-activation, so that we can more effectively combine transitions.

Our study of the smoothed Rényi divergences also brought up new questions. Even though we managed to find a region for ϵ for which there exists a steepest state, this region is still quite small in some scenarios. Especially when dealing with states of infinite dimension, this can become a problem. For such states, this means that no steepest state can be found. Thus, it is desirable that these restrictions are made less stringent.

As we showed in one of the examples, however, when the restrictions on ϵ are not met, we can possibly find examples of states that are incomparable with the steepest state. Thus, the most feasible way to solve this problem, is probably to take catalysts into account. Using catalysts, we can possibly make these incomparable states comparable. In the ideal case, this could then be used to define a steepest state that is, when taking catalysts into account, the steepest state for any ϵ.

Another solution strategy could be to define a new smoothed divergence based on these steepest and flattest states. Instead of maximizing and minimizing the Rényi divergences for states within an ϵ-ball, we could instead use the Rényi divergences of the steepest and flattest states respectively. Then, these quantities might share a lot of the useful properties with the smoothed Rényi divergences.

This does create new problems, though these might be easier to solve than the original problem. It seems that this strategy would require a steepest state to be defined for all ϵ. This is not necessary, however. Instead, we could approximate the steepest state outside of the region for which we can find one.

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