Correlations in mediated dynamics

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Abstract

In a plethora of physical situations one can distinguish a mediator—a system that couples other, non-interacting systems. In this thesis, we analyze such scenarios from a quantum information theory standpoint by exploring the relation between correlations and mediated dynamics. We start with a unified description of various types of correlations in the context of resource theories. Then we concentrate on negativity, which is distinguished as one of the few computable entanglement monotones. We construct a hierarchy of distance-based correlation measures that are comparable to negativity. Then we study the correlations in two probes interacting via a mediator. We define classical interactions through commutativity of the interaction Hamiltonians. We propose methods to detect nonclassicality of the interaction solely through the correlations in the probes. Finally, we discuss applications of this formalism to restrict possible theories of gravity in a Hilbert space and to the theory of quantum simulators.

Streszczenie

W wielu układach fizycznych można wyróżnić pośrednika — podukład, który sprzęga inne, bezpośrednio nieoddziałujące ze sobą podukłady. Niniejsza rozprawa poświęcona jest analizie dynamiki z pośrednikiem z punktu widzenia kwantowej teorii informacji, ze szczególnym uwzględnieniem korelacji. Rozpoczynamy od unifikacji różnych rodzajów korelacji w ramach ogólnej teorii zasobów. Następnie skupiamy się na tzw. ujemności, gdyż spośród wielu miar splątania wyróżnia ją łatwość obliczania. Wprowadzamy hierarchię różnych form korelacji, opartych na pojęciu odległości, które można bezpośrednio porównać do ujemności. Następnie stosujemy te i inne miary korelacji w układzie dwóch próbek oddziałujących przez pośrednika. Definiujemy klasyczne oddziaływania poprzez komutację Hamiltonianów oddziaływania pomiędzy każdą próbką i pośrednikiem. Następnie wprowadzamy metody wykrywania nieklasycznych oddziaływań wyłącznie za pomocą korelacji pomiędzy próbkami. Na koniec opisujemy zastosowanie tych metod do ograniczenia możliwych teorii grawitacji w przestrzeni Hilberta i do kwantowych symulatorów.

Publications

Many of the results, ideas, and figures contained in this thesis have been published in the following articles:

- [KGL+18]: Detecting nondecomposability of time evolution via extreme gain of correlations

  Tanjung Krisnanda, Ray Ganardi, Su-Yong Lee, Jaewan Kim, Tomasz Paterek

  Phys. Rev. A **98** 052321 — Published 16 November 2018

- [GMPZ22]: Hierarchy of correlation quantifiers comparable to negativity

  Ray Ganardi, Marek Miller, Tomasz Paterek, Marek Żukowski

  Quantum **6**, 654 (2022) — Published 16 February 2022

- Quantitative nondecomposability of unknown mediated dynamics

  Ray Ganardi, Mahasweta Pandit, Ekta Panwar, Bianka Wołoncewicz, Tomasz Paterek

  Manuscript in preparation

My other publications that are not included in this thesis

- Entanglement gain in measurements with unknown results

  Margherita Zuppardo, Ray Ganardi, Marek Miller, Somshubhro Bandyopadhyay, Tomasz Paterek

  Phys. Rev. A **99** 042319 — Published 10 April 2019

- Generalised uncertainty relations from superpositions of geometries

  Matthew J. Lake, Marek Miller, Ray Ganardi, Zheng Liu, Shi-Dong Liang, Tomasz Paterek

  Class. Quantum Grav. **36** 155012 — Published 17 July 2019

- Cooperation and dependencies in multipartite systems

  Waldemar Kłobus, Marek Miller, Mahasweta Pandit, Ray Ganardi, Lukas Knips, Jan Dziewor, Jasmin Meinecke, Harald Weinfurter, Wiesław Laskowski, Tomasz Paterek

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Notation

We shall use the following notation:

Symbol	Definition
$\mathcal{H}$	Hilbert space
$\mathcal{D}$	set of density matrices
$\mathcal{S}$	set of free states
$\mathcal{F}$	set of free operations
$\mathbb{1}$	identity map, or identity matrix
$\{\|i\rangle\}$	computational basis
$\{\|e_i\rangle\}$	basis
$\|\psi\rangle$	pure quantum state
$\|\Phi\rangle$	maximally entangled state, $\|\Phi\rangle = \sum_i \frac{1}{\sqrt{d}} \|ii\rangle$
ρ, σ	quantum states
ψ	density matrix of a pure quantum state, $\psi = \|\psi\rangle \langle\psi\|$
$\mathrm{Tr}\, X$	trace of the operator X
$\mathrm{Tr}_A\, X_{AB}$	partial trace over A, $\mathrm{Tr}_A\, X_{AB} = \sum_i (\langle i\| \otimes \mathbb{1})\, X_{AB}\, (\|i\rangle \otimes \mathbb{1})$
$T_A(X)$	partial transposition in the computational basis of subsystem A, $T_A(X) = \sum_{ij} (\|i\rangle \langle j\| \otimes \mathbb{1}) X (\|j\rangle \langle i\| \otimes \mathbb{1})$
$\|X\|$	absolute of the operator X, $\|X\| = \sqrt{X^\dagger X}$
$(X)_+$	positive part of operator X, $(X)_+ = \frac{1}{2}(X + \|X\|)$
$(X)_-$	negative part of operator X, $(X)_- = \frac{1}{2}(X - \|X\|)$
$\\|X\\|_1$	trace norm
$\\|X\\|_\infty$	spectral norm
$\\|X\\|_\alpha$	Schatten norm of order α, $\\|X\\|_\alpha = (\mathrm{Tr}\, \|X\|^\alpha)^{1/\alpha}$
$d_{tr}(\rho, \sigma)$	trace distance, $d_{tr}(\rho, \sigma) = \frac{1}{2}\\|\rho - \sigma\\|_1$
$S(\rho\\|\sigma)$	quantum relative entropy, $S(\rho\\|\sigma) = \mathrm{Tr}\, \rho(\log\rho - \log\sigma)$
$d_T(\rho, \sigma)$	partial transpose distance, $d_T(\rho, \sigma) = \frac{1}{2}\\|T_A(\rho) - T_A(\sigma)\\|_1$
$PROD$	set of product states
CC	set of classically correlated states, $CC = \{\sum_i p_i \|e_i f_i\rangle \langle e_i f_i\|\}$
QC	set of quantum-classical states, $QC = \{\sum_i p_i \rho_i \otimes \|e_i\rangle \langle e_i\|\}$
SEP	set of separable states
PPT	set of states that are positive under partial transposition

Contents

Chapter 1

Introduction

Today, we believe that all physical theories satisfy the locality principle. Roughly stated, the principle says "two space-like separated events must be independent." The main motivation behind the acceptance of this principle comes from the success of special relativity and experimental observation of retardation of physical interactions.

Although intuitive, locality combined with other properties produces counter-intuitive consequences. For example, the EPR paradox [EPR35] comes from the interplay between locality, quantum theory, and hidden variables—or as Einstein called it "elements of reality". As we strongly believe in locality and quantum theory has passed many experimental tests, this necessitates us to reject local hidden variable models.

However, we do see distant objects interact in the real world. How is their interaction modeled within physical theories satisfying locality? Classical physics resolves this by postulating the existence of a field, permeating through space, acting as the "mediator" of the interaction. As a result, distant objects that interact only locally with the field admit an effective interaction mediated by changes in the field.

The situation in quantum theory does not differ much—we just promote the fields to operators. Effectively, it is as if there is a quantum object that is delocalized in space that mediates the interaction between two other objects. Let us state this formally. Suppose we have two quantum objects A, B that interact via a mediator M. Assuming that the system is closed—which can be ensured by considering purifications—the dynamics of the system is governed by a Hamiltonian of the form $H = H_{AM} + H_{BM}$. The state of the system evolves according to the usual unitary evolution $\rho_t = e^{-itH}\rho_0 e^{itH}$ (throughout this thesis, we will set $\hbar = 1$).

One might ask, what happens when the mediator is a classical system? To answer this, first we must define what it means for a mediator to be classical. There are many different proposals on how to define classicality of a quantum system [PT01, Ter06, HR18]. In this thesis, we define classicality by commutativity—a quantum system is classical if all of its observables commute. Therefore, a classical mediator is a mediator whose coupling to other systems commute, i.e. $[H_{AM}, H_{BM}] = 0$. This is consistent with the defining feature of quantum systems, that there exists observables that *do not* commute.

Of course, this is not the only possible notion of nonclassicality. It is entirely possible to define classical interactions through, for example, the operator Schmidt rank. Recall that any bipartite operator X can always be written as a linear combination of product operators, $X = \sum_{i=1}^{r} A_i \otimes B_i$. The operator Schmidt rank of an operator is the smallest r among all such decompositions [MHN18]. We can define classical interactions as those interactions that have operator Schmidt rank 1, i.e. they are of the form $A \otimes B$. Therefore, within this definition, it is possible for the interaction with a single object and the mediator to be nonclassical—for example the interaction $X_A X_M + Y_A Y_M$ has operator Schmidt rank 2. However, when the interaction term has operator Schmidt rank 1, say $A \otimes B$, the interaction between two objects of the same kind with the mediator must commute $[A_1 \otimes B, A_2 \otimes B] = 0$.

This shows that interactions that are classical in the operator Schmidt rank sense must also be classical in the commutative sense.

An important motivation to study the classicality of mediated dynamics comes from the possibility of observing nonclassical features of gravitational interaction between massive objects [BMM$^+$17, MV17]. In order to provide meaningful restrictions on quantum theories of gravity, we need to formulate a method that makes minimal assumptions about the quantum model of the gravitational field. This is because it is still unclear how to quantize gravity, with different proposals having different problems [DB22, HR18]. Yet, there is one feature that these proposals have in common: they are all local theories—each particle only interact with the gravitational field at a point, not globally. In some proposals, there is also a Hilbert space associated with the gravitational field. Although these theories resemble standard quantum mechanics, there is an added difficulty due to the inaccessibility of the gravitational subsystem. We aim to fill exactly this gap.

The essential goal of this thesis is the study of the quantumness of the mediator assuming that we do not have access to the mediating system experimentally. To do this, we will examine the correlations between A and B when we assume that the mediator M is classical. We will show that if the dimension of the mediator M is bounded, then the maximum correlation that A and B can obtain is also bounded above. We will show that this bound *can* be violated if the mediator is nonclassical. Furthermore, we will show that the violation of this bound gives a lower bound on a distance to the set of maps implementable with a classical mediator. We will also give a simple lower bound on the norm of the commutator of interaction terms, and give generalizations of these bounds to open systems.

1.1 Why correlations?

Given the definition of nonclassicality as non-commutativity, we define classically mediated interactions as those interactions whose couplings to the mediator commute. Note that this notion of classicality of interactions is inherently multipartite—it does not make sense to ask whether the interaction of a single object and the mediator is classical or not. When there is only a single object A coupled to the mediator M, there is only *one* interaction term H_{AM}, so of course $[H_{AM}, H_{AM}] = 0$. Thus, it is natural to consider two objects interacting via the mediator.

There have been indications that we can detect nonclassicality through the correlations between two objects. Consider the formalism of quantum field theory in curved spacetime, where the gravitational field is modeled as a background metric to the quantum fields. It is known that some information about the metric is imprinted into the propagators of the quantum fields [SAK16]. It is widely accepted that for quantum fields, propagators are a measure of correlation. In fact, this imprinted information is sufficient to reconstruct the metric from the correlations.

A more suggestive indication comes from the problem of entanglement distribution or more broadly of quantum communication—two parties A, B would like to obtain some correlation by sending a small "mediator" system M from one laboratory to the other. See Figure 1.1 for illustration. The gain of entanglement in one round of exchange is then the difference between the final entanglement $E_{A:MB}(\rho)$ when the mediator M is in the laboratory together with system B and the initial entanglement $E_{AM:B}(\rho)$ before M is transmitted. If entanglement is measured by the relative entropy of entanglement [VPRK97], it was shown that the gain in entanglement is bounded by the discord $D_{AB|M}(\rho)$ [SKB12, CMM$^+$12], i.e. $|E_{A:MB}(\rho) - E_{AM:B}(\rho)| \leq D_{AB|M}(\rho)$. Therefore, any observation of entanglement gain between the laboratories caused by the exchange of the mediator M must mean $D_{AB|M} > 0$. Since $D_{AB|M}(\rho)$ quantifies the distance from ρ to the set of states where M is classical, we conclude that in this scenario entanglement gain certifies that the mediator is nonclassically correlated to the other systems. Here, classicality of a state means it is possible to write the total tripartite state using the states of only one basis in the Hilbert space

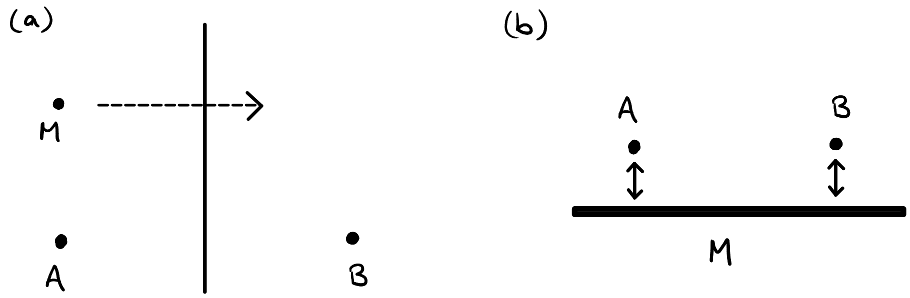

Figure 1.1: Discrete exchange of mediator vs. continuous. In (a), the interaction is relayed through a discrete exchange of a mediator system M. In (b), the interaction is relayed by continuous coupling to a mediator system M.

of M, i.e. $\rho_{ABM} = \sum_i p_i \rho^i_{AB} \otimes |e_i\rangle\langle e_i|_M$, where p_i's are probabilities, ρ^i_{AB} are quantum states on AB and $\{|e_i\rangle_M\}$ forms a basis of $\mathcal{H}_M$. This result has also been extended to continuous-in-time dynamics: Ref. [KZPP17, PBK+21] showed that if the discord $D_{AB|M}$ is zero throughout the dynamics, then entanglement $E_{A:BM}$ cannot increase. A weaker, but fascinating formulation is also provided—if $D_{AB|M}$ is zero throughout the dynamics, then $E_{A:B}(t) \leq S^0_A + S^0_B$. Here $S^0_{A,B}$ denotes the von Neumann entropy of the initial state. This demonstrates the possibility of inferring something about the classicality of the mediator—in this case discord—even though we do not have access to it. Furthermore, the exact form of the coupling between the probes A, B and the mediator M is left unknown, so the formalism is applicable to uncharacterized systems. Note that this is a different notion of classicality from our definition. In these works, the classicality lies in the state instead of the interaction.

Although different, the classicality of the state and of the interaction are closely related. By definition, a state has zero discord $D_{AB|M}(\rho_{ABM})$ if and only if there exists a rank-1 projection π_M acting on subsystem M such that $\pi_M(\rho_{ABM}) = \rho_{ABM}$. When the state has zero discord throughout the dynamics, then we can find π^t_M such that $\rho^t_{ABM} = \pi^t_M(\rho^t_{ABM})$. Note that these projectors π^t_M can be different at different times. Now, suppose the rank-1 projection π^t_M is time-independent, i.e. $\pi^t_M = \pi_M$. Then, the Hamiltonian $H' = \pi_M(H_{AM}) + \pi_M(H_{BM})$ produces the same evolution as the original Hamiltonian $H = H_{AM} + H_{BM}$. This is because Lemma 1.1 implies that $\pi_M(\rho^t_{ABM}) = \rho^t_{ABM}$ together with $\pi_M([H, \rho^t_{ABM}]) = [H, \rho^t_{ABM}]$ implies $[H, \rho^t_{ABM}] = [\pi_M(H), \rho^t_{ABM}] = [H', \rho^t_{ABM}]$. This modified Hamiltonian has the additional property that the interaction terms commute, and therefore the mediator is classical in the commutative sense.

Lemma 1.1. *Let X_{AB}, Y_{AB} be linear operators acting on $\mathcal{H}_A \otimes \mathcal{H}_B$, and*

$$\Pi_B(Z) = \sum_i |e_i\rangle\langle e_i| Z |e_i\rangle\langle e_i| \tag{1.1}$$

a rank-1 projective map, where $\{|e_i\rangle\}$ forms a basis of $\mathcal{H}_B$.

If

$$(\mathbb{1}_A \otimes \Pi_B)(Y_{AB}) = Y_{AB}, \text{ and} \tag{1.2}$$

$$(\mathbb{1}_A \otimes \Pi_B)([X_{AB}, Y_{AB}]) = [X_{AB}, Y_{AB}], \tag{1.3}$$

then $[X_{AB}, Y_{AB}] = [(\mathbb{1}_A \otimes \Pi_B)(X_{AB}), Y_{AB}]$.

Proof. Let us write X_{AB}, Y_{AB} in the following block form

$$X_{AB} = \sum_{ij} X_{ij} \otimes |e_i\rangle \langle e_j| , \tag{1.4}$$

$$Y_{AB} = \sum_{ij} Y_{ij} \otimes |e_i\rangle \langle e_j| , \tag{1.5}$$

where X_{ij}, Y_{ij} are linear operators acting on $\mathcal{H}_A$. Eq. (1.2) implies that Y_{AB} is block diagonal, i.e. $Y_{AB} = \sum_k Y_{kk} \otimes |e_k\rangle \langle e_k|$. Computing the commutator, we have

$$\begin{aligned}
[X_{AB}, Y_{AB}] &= \left[\sum_{ij} X_{ij} \otimes |e_i\rangle \langle e_j| , \sum_k Y_{kk} \otimes |e_k\rangle \langle e_k| , \right] && (1.6)\\
&= \sum_{ij} (X_{ij} Y_{jj} - Y_{ii} X_{ij}) \otimes |e_i\rangle \langle e_j| . && (1.7)
\end{aligned}$$

However, Eq. (1.3) implies that $[X_{AB}, Y_{AB}] = \sum_l Z_l \otimes |e_l\rangle \langle e_l|$ for some matrices Z_l, i.e. the commutator must be block diagonal. Therefore, we must have $X_{ij}Y_{jj} - Y_{ii}X_{ij} = 0$ if $i \neq j$. This leaves us with

$$\begin{aligned}
[X_{AB}, Y_{AB}] &= \sum_{ij} (X_{ij} Y_{jj} - Y_{ii} X_{ij}) \otimes |e_i\rangle \langle e_j| . && (1.8)\\
&= \sum_{i} (X_{ii} Y_{ii} - Y_{ii} X_{ii}) \otimes |e_i\rangle \langle e_i| && (1.9)\\
&= \sum_{i} [X_{ii}, Y_{ii}] \otimes |e_i\rangle \langle e_i| && (1.10)\\
&= \left[\sum_{i} X_{ii} \otimes |e_i\rangle \langle e_i| , \sum_j Y_{jj} \otimes |e_j\rangle \langle e_j| \right] && (1.11)\\
&= [(\mathbb{1}_A \otimes \Pi_B)(X_{AB}), Y_{AB}] , && (1.12)
\end{aligned}$$

which proves the claim. □

Therefore we see that in some cases, classicality of the state implies classicality of the interaction. In this thesis, we will extend this line of research to study the quantumness of the interaction, instead of the joint state of the systems.

1.2 Why (quantum) mediators?

Since physical interactions are defined by the behavior of the mediator, studying the mediator allows us to conclude some things about the interactions themselves. The canonical example is the study of the interaction between matter and light fields, resulting in the formulation of the theory of quantum electrodynamics. For the past few decades, we witnessed many extensions of quantum theory to incorporate gravity, but proposed experiments testing these theories are mostly out of the reach of current experimental capabilities [DB22, CBPU19]. Recently, there is an interest in bringing techniques from quantum information to provide predictions testable on table-top experiments that can invalidate some models of quantum gravity [BMM+17, MV17, KZPP17]. With the advance of control over massive systems [Asp22], such table-top gravitational experiments are reaching feasibility. Therefore, with further development of methods to test nonclassicality of mediators, we can put further constraints on the quantum nature of gravity.

Besides answering foundational questions, there are also more modest implications of this study. As a motivating example, let us examine a quantum optics setup. Suppose systems A, B, M are single mode light fields. The interaction Hamiltonian is given by $H = a_A^\dagger a_M + a_B^\dagger a_M +$ h.c., where $a, a^\dagger$ are the ladder operators. Furthermore, suppose the initial state shared by AB is in a product state with M, with a coherent state at M, i.e. $|\psi_0\rangle = |\psi_{AB}\rangle \otimes |\alpha_M\rangle$. If the amplitude of the state at M is very large, i.e. $\alpha_M \gg 1$, then $a_M^\dagger |\alpha_M\rangle \approx \alpha_M^* |\alpha_M\rangle$, and effectively the interaction can be described by the Hamiltonian $H = a_A^\dagger \alpha_M + a_B^\dagger \alpha_M +$ h.c.. This is exactly the Hamiltonian that describes two quantum fields A, B interacting with a *classical* field M. Notice that the Hamiltonian splits into two local parts, so effectively the whole evolution is described by a local unitary acting on A and separately a local unitary on B. Because correlations must be monotonic under local operations, the correlation between A and B cannot increase. Therefore, to distribute entanglement through a light field, the amplitude at the mediator M cannot be too large—otherwise we cannot even correlate A and B. We can understand this phenomenon as a continuous interaction analogue of the paradigm of local operations and classical communication (LOCC)—quantum systems cannot get entangled by classical communication.

Another application is in the quantum simulation of many-body systems. Suppose we have a quantum simulator—a quantum system that we can control to some degree—and we would like to simulate a many body system with N-parties. We do this by applying a series of gates to our simulator, such that the resulting map is equivalent to the evolution of the many-body system. In general, simulating a system with an arbitrary Hamiltonian necessitates an exponential amount of resources, making the problem intractable. Fortunately, the Hamiltonian for most systems of interest is k-local—that is, the Hamiltonian if of the form $H = \sum_i H_i$, where each H_i term acts on at most k-subsystems. The restricted problem of simulating k-local Hamiltonians turns out to be much simpler than the general one—it is even tractable [Llo96]. Recent results [CST$^+$21] show that the error in simulating a k-local Hamiltonian is asymptotically bounded by the sum of the norm of N nested commutators $\sum_{a_1,\ldots,a_N=1}^{N} \|[H_{a_N}, \ldots, [H_{a_2}, H_{a_1}]]\|_\infty$. In this context, we are studying the correlation in the simplest systems with 2-local Hamiltonians, and its relation to the commutators $[H_i, H_j]$. Since our result provides a lower bound on the norm of the commutator of interaction terms, this bounds the asymptotic error scaling in simulating N-body dynamics described by a 2-local Hamiltonian.

1.3 Summary of results

These examples show that the physics of mediators is incredibly rich, and has broad applicability to a number of problems. We will explore these issues in the following chapters.

In Chapter 2, we discuss the theory of correlations. We start by reviewing the framework of resource theories and propose a definition of resource theory of correlations. We continue by defining correlation measures as resource monotones and review typical constructions of correlation measures. We show that these definitions are consistent with the correlation measures typically used in the literature, with some caveats on quantum discord. We finish by commenting on computability of these measures.

Chapter 3 discusses negativity and its relation to distance-based correlation measures. We show that we can define a distance—we call it the partial transpose distance—on the set of states, such that correlation measures based on this distance are comparable to negativity. We conjecture that negativity is in fact equal to the partial transpose distance to PPT states and provide supporting evidence. This allows us to fairly compare negativity to measures of other types of correlations, because they are constructed from the same distance. We close this chapter by investigating the geometry of correlations with partial transpose distance, and show a subadditivity relation for total correlations in a pure state. This chapter is based on the results presented in Ref. [GMPZ22].

Chapter 4 discusses mediated dynamics, where we have two systems A, B whose interaction is relayed through a mediator M. We start by defining classical interactions and relate them to a decomposability property of maps. We provide a necessary criterion for correlations in decomposable dynamics and show examples of violation of this criterion, witnessing the nondecomposability of the dynamic. We extend this analysis to the scenario where the mediator is inaccessible, in view of restricting quantum theories of gravity. More specifically, we formulate a necessary condition for a map to have a decomposable dilation, phrased only in terms of correlations between A and B and the dimension of M. This condition is independent of the actual coupling to the mediator, making it suitable for scenarios where we do not have a full characterization of the dynamics. We then define measures of nondecomposability along with methods to estimate lower bounds from the violation of these criteria. We close by discussing the implications for the theory of quantum simulators and the Bose-Marletto-Vedral experiment. This chapter is partially based on the results presented in Ref. [KGL$^+$18].

Chapter 2

Correlations

Poincaré said that mathematics is the art of giving the same name to different things [Poi18]. True to the quote, there exist many different definitions of what correlations are—a statistician would say covariance quantifies the correlation between two random variables, but an information theorist would say we should quantify it by mutual information. Quantum theory does not help to clarify the situation, instead it exacerbates the problem—we get even more notions of correlations. For example, some people call the conditional probability of outcomes that you get in a Bell scenario as correlation. If you talk to people working with quantum field theories, they will talk about (n-point) correlation functions. A quantum information theorist says correlations truly exist *within* quantum states, and they take various forms such as entanglement, discord, dissonance, etc.

Reflecting back on the quote, there is something unifying these different things. After all, there is an art to the name-giving. In this chapter, we will explore what we mean by correlation measures, review some common constructions, and comment on some aspects of computability. We will draw heavily from the resource theoretic perspective presented in Ref. [CG19] while noting the special details that make it a theory of *correlations* instead of resources.

2.1 Resource theory and correlations

In this thesis, when we say correlations we mean the correlation that is contained in a quantum state. For simplicity, consider a bipartite system with Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$. Suppose the system is in some state ρ, and we have two local observables O_A, O_B. By correlation in a quantum state, we mean the statistical relation between the measurement outcomes of O_A and O_B. When we only have one local observable for each subsystem, then the relation can be described by classical probability theory—there exists a joint probability distribution that describes the outcomes. Furthermore, we can always choose this joint probability distribution to be local—the measurement outcome at A does not depend on B except indirectly through some local hidden variable. Such a joint probability distribution is also called a local hidden variable model. However, if we consider the correlations in at least two local observables for each subsystem, this is not necessarily true. This is the point of Bell's theorem [Bel64]—for some quantum states, we cannot reproduce the correlation between measurement outcomes with local hidden variable models. In other words, while for any pair of local observables the joint probability clearly exists, it cannot be extended to a joint probability of outcomes for all observables. It was found that these "stronger-than-classical" correlations are related to entanglement [Wer89].

Since entanglement was the first example of a kind of correlation that is only exhibited in quantum systems, for a long time it was equated with *all* quantum correlations. Part of the reason is that for bipartite pure states, all correlations take the same form—if a pure state is correlated (not product), then it must be entangled. However, over the years we have learned

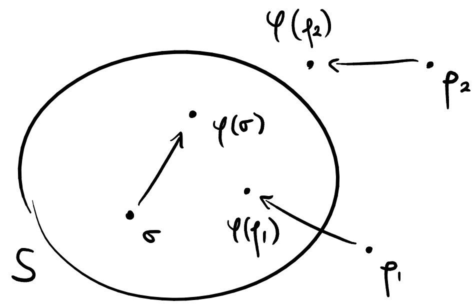

Figure 2.1: Illustration of a resource theory. A free operation $\varphi \in \mathcal{F}$ must map a free state $\sigma \in \mathcal{S}$ to another free state $\varphi(\sigma) \in \mathcal{S}$. A resourceful/non-free state can be mapped to either a free state (as for ρ_1) or a non-free state (as for ρ_2). In a resource theory of correlations, we identify the set of uncorrelated states as the free states and a physically-motivated subset of non-correlating operations as the free operations.

that separable states can also exhibit nonclassical forms of correlations, e.g. discord [HV01, OZ01, Zur00]. Today, we understand that correlations in a quantum state can take many forms, including total correlation [GPW05, MPS⁺10], discord [MBC⁺12, BDS⁺17], entanglement [HHHH09], steering [GA15], and Bell-nonlocality [WSS⁺20] among others. These different forms of correlations are useful in different ways—entanglement allows us to teleport quantum states [BBC⁺93], while Bell-nonlocality is linked to an advantage in certain communication tasks [BŻPZ04, BCMdW10].

With these developments, some patterns emerged in different theories of correlations. Namely, correlations behave like resources that can be manipulated. An abstraction of these resource manipulations lead to the formulation of resource theory [CG19]. Today, we understand correlations as a special type of resource theory. The resource theory that is associated with a correlation is one whose free states are the uncorrelated states and whose free operations are a set of physically-motivated operations that do not correlate the systems. For example, we understand entanglement as a resource theory where the free states are the separable states and the free operations are the LOCC maps [Wer89, HHHH09].

However, not all resource theories are about correlations. For example, it is hard to think of coherence [SAP17] or resource theory of quantum thermodynamics [GHR⁺16, GMN⁺15] as correlation—there is only a single system involved in these scenarios. A theory of correlations must be a resource theory with some multiparty structure.

To formulate this point precisely, let us review the basic notions in a resource theory (see Figure 2.1).

Definition 2.1. A *resource theory* $(\mathcal{S}, \mathcal{F})$ consists of a set of free states $\mathcal{S} \subseteq \mathcal{D}$ and a set of free operations $\mathcal{F}$ such that

1. $\mathbb{1} \in \mathcal{F}$.
2. $\mathcal{F}$ is closed under composition.
3. For all $\varphi \in \mathcal{F}$, we have $\varphi(\mathcal{S}) \subseteq \mathcal{S}$.

Example 2.1. 1. Entanglement: the free states are separable states and the free operations are LOCC maps [Wer89, HHHH09].

2. Coherence: the free states are incoherent states and the free operations are incoherent operations [SAP17].

3. Discord: the free states are classical-quantum states and the free operations are classical-quantum operations [MBC+12, BDS+17].

4. Total correlations: the free states are product states and the free operations are product maps [GPW05, MPS+10].

5. PPT entanglement: the set of free states are PPT states and the free operations are PPT operations [Rai99, Rai01].

6. Steering: the set of free states are unsteerable assemblages and the free operations are one-way LOCC [GA15].

The multipartite structure is expressed by resource theories that admit a tensor product structure [CG19].

Definition 2.2. A resource theory $(\mathcal{S}, \mathcal{F})$ *admits a tensor product structure* if:

1. All free operations are completely free, i.e. for all $\varphi \in \mathcal{F}_{\mathcal{X}\to\mathcal{Y}}$, we have $\mathbb{1}_{\mathcal{Z}} \otimes \varphi \in \mathcal{F}_{\mathcal{Z}\mathcal{X}\to\mathcal{Z}\mathcal{Y}}$.

2. Appending free states is a free operation, i.e. for all $\sigma \in \mathcal{S}_{\mathcal{Y}}, \varphi_\sigma(\rho) = \rho \otimes \sigma$, we have $\varphi_\sigma \in \mathcal{F}_{\mathcal{X}\to\mathcal{X}\mathcal{Y}}$.

3. Discarding a subsystem is a free operation, i.e. $\mathrm{Tr}_{\mathcal{X}\mathcal{Y}\to\mathcal{X}} \in \mathcal{F}_{\mathcal{X}\mathcal{Y}\to\mathcal{X}}$.

The relevance of these conditions to a theory of correlations is evident. Condition 1 says that applying a free operation to a correlated subsystem is still a free operation. Conditions 2 and 3 combined mean that we can freely create and discard free states. All resource theories shown in Example 2.1 admit a tensor product structure.

However, we already argued that coherence should *not* be a correlation. The missing ingredient is this—correlation is the separation between the actual state and something that can be produced from an uncorrelated state by acting locally on each subsystem and some permitted version of collaboration. For example, we say a state is entangled if we *cannot* reproduce the state by applying some LOCC map to a separable state. This means that for any resource theory of correlation, the set of free operations must include all product maps—otherwise we can *create* correlation by performing some local operation. Since some local operations are not free in the resource theory of coherence, it cannot be a theory of correlation. We propose the following definition for a *resource theory of correlation*:

Definition 2.3. A resource theory $(\mathcal{S}, \mathcal{F})$ is a *theory of correlation* if it admits a tensor product structure and the set of free operations includes all product maps.

Most of the examples above—entanglement, PPT entanglement, and total correlations—fulfill this definition. The difference is only in the allowed type of collaboration—entanglement allows classical communication, whereas total correlation does not allow any collaboration. However, the resource theory of quantum discord does not satisfy Definition 2.3. We know that discord quantifies how far is our system from a classical-quantum description. However, we can increase the discord in a state by performing a quantum operation on the classical part. By our definition, the resource theory of discord is *not* a theory of correlation.

Another notable example of a theory that is excluded by Definition 2.3 is the resource theory of Bell nonlocality. Suppose we define a resource theory of Bell nonlocality by saying the free operations are LOCC, and the free states are those states that do not exhibit Bell nonlocality. It is known that this resource theory exhibits superactivation—there are states ρ, σ that are free, yet $\rho\otimes\sigma$ is not [Pal12]. This implies appending free states is not necessarily a free operation, which means it does not admit any tensor product structure.

2.2 Correlation measures

Since correlation can be seen as a special form of resource, we can use the standard techniques in the formalism. A standard way to quantify the amount of resource in a state is through the use of resource monotones.

Definition 2.4. A *resource monotone* for a given resource theory $(\mathcal{S}, \mathcal{F})$ is a function $Q : \mathcal{D} \to \mathbb{R}$ such that for any state ρ and any free operation $\varphi \in \mathcal{F}$, we have $Q(\rho) \geq Q(\varphi(\rho))$.

Initially, monotones are formulated in the context of the transformability problem—given ρ, σ, is there a free operation $\varphi \in \mathcal{F}$ such that $\varphi(\rho) = \sigma$? If there exists a resource monotone Q such that $Q(\sigma) > Q(\rho)$, then we know such a transformation is impossible. Note that the ordering imposed by different monotones might not be unique—we might have $Q_1(\rho) > Q_1(\sigma)$ and $Q_2(\rho) < Q_2(\sigma)$. This is already shown for several entanglement measures [VP00, MG04]. We relate this definition to correlation measures as follows:

Definition 2.5. A *correlation measure* is a resource monotone for some theory of correlation.

Note that this definition elevates monotonicity as the essential property of correlation measures—although other properties discussed in the literature such as positivity, faithfulness, convexity, additivity, and continuity are useful, they are of secondary importance. From this definition, we can already show that for a correlation measure must be *constant* on the set of uncorrelated states. If we set this constant to be zero, then the resulting measure will be positive.

In the literature, there are many different measures of correlation [HHHH09, MBC+12, CG19]. However, we can understand the broad categories by looking at several common constructions. Since entanglement theory is one of the most widely studied resource theory, many of these measures were first defined for entanglement. Often, the construction can be generalized to other types of correlations.

2.2.1 Information theoretic measures

Information theory is fundamentally a theory of information processing tasks [CT05]. One of the basic problems is the following—suppose we have a noisy channel, what is the optimal rate of transmission through this channel? Superficially, it is very similar to the basic task in resource theory—what is the optimal rate of transformation between two states? Thus, we will call measures that stem from rates of information processing tasks as information theoretic measures.

As stated before, initially resource monotones were used to detect the impossibility of a certain transformation under free operations. One of the first examples was in the theory of entanglement measures. For pure bipartite states, the conditions for the possibility of LOCC transformations are known [Nie99]. In addition, there exists a collection of measures that fully characterize the possible transformations for pure states [Vid99]. The measures are defined as follows—let $|\psi\rangle = \sum_i \sqrt{p_i}\,|e_i f_i\rangle$ be a pure state in its Schmidt basis, with p_i ordered from largest to smallest. We define E_k to be the sum of the $(d-k)$-smallest Schmidt coefficients $E_k(\psi) = \sum_{i>k} p_i$. Then there is an LOCC transformation that takes ψ to φ if and only if $E_k(\psi) \geq E_k(\varphi)$ for all k.

This characterization implies that there exists a maximally entangled state—a state that maximizes the entanglement measure. The maximally entangled state is a pure state whose Schmidt coefficients are all equal: $|\Phi\rangle = \sum_i \frac{1}{\sqrt{d}}\,|e_i f_i\rangle$. More interestingly, because this set of monotones completely characterizes the possible transformations, we can transform the maximally entangled state to *any* pure state. When we have many copies of a state, we can also concentrate the entanglement into some smaller number of maximally entangled states. This phenomenon is known as entanglement distillation [BBPS96, BDSW96, BBP+96].

Entanglement cost is an entanglement measure that is related to the phenomenon of quantum teleportation [BBC+93, BBP+96, BBPS96, BDSW96, PV07]. Recall the scenario—Alice and Bob share a Bell state Φ and Alice would like to send a qubit in the state ρ. Alice performs a joint measurement on both qubits in her possession, and communicates the outcome classically to Bob. Bob then applies a unitary correction that depends on Alice's outcome and the final state of the qubit in his lab will be ρ. By using multiple copies of Bell states, the protocol can be adapted to send higher-dimensional systems. This means that with LOCC operations, Alice and Bob can prepare *any* quantum state if they have an unlimited supply of Bell states—Alice can simply prepare the full state in her lab, then send one part to Bob through the teleportation protocol. However, this is not optimum because we would need $\log d_B$ Bell pairs to create every state, whereas we know that preparing product states can be done without using up any Bell pairs at all. The entanglement cost $E_C(\rho)$ is defined as the minimum asymptotic rate of entanglement needed to prepare ρ

$$E_C(\rho) = \lim_{\varepsilon \to 0, n \to \infty} \sup\{m/n \,|\, d_{tr}\left(\rho^{\otimes n}, \varphi_m(\Phi^{\otimes m})\right) \leq \varepsilon, \varphi_m \text{ LOCC}\}, \tag{2.1}$$

where we start with m Bell states and obtain n copies of ρ. The dual measure—distillable entanglement—measures the maximum asymptotic rate of entanglement that we can distill

$$E_D(\rho) = \lim_{\varepsilon \to 0, n \to \infty} \sup\{m/n \,|\, d_{tr}\left(\varphi_n(\rho^{\otimes n}), \Phi^{\otimes m}\right) \leq \varepsilon, \varphi_n \text{ LOCC}\}, \tag{2.2}$$

when we start with n copies of ρ and obtain m copies of Bell states. From the definitions, it is easy to see that these quantities are resource monotones for entanglement theory. However, they are generally not equal, as shown recently in Ref. [LR21].

These quantities can also be defined in other resource theories that admit a *golden unit*—a state that serves as a unit of resource. The crucial property is that given an unlimited supply of golden units, the restriction to free operations is lifted and we can prepare any state.

2.2.2 Convex roof measures

For many measures, it is easy to define and compute them for pure states and rather difficult at first glance to extend their definitions to mixed states (e.g. the Schmidt rank). However, there are many schemes to extend a function on pure states to mixed states. A particularly common construction is the "convex roof" extension, because the correlation measure obtained will be convex. Furthermore, if the correlation measure is asymptotically continuous on pure states, then the extension automatically inherits this property. Monotonicity also follows automatically from monotonicity on pure states. In fact, it is characterized by being the largest measure among all convex measures that take the same value on pure states [Uhl98]. This means that the convex roof extension $\tilde{f}(\rho)$ of a measure $f(\psi)$ satisfies

$$\tilde{f}(\rho) = \sup_{\substack{g(\psi)=f(\psi), \\ g(\sum_i p_i \rho_i) \leq \sum_i p_i g(\rho_i)}} g(\rho). \tag{2.3}$$

The canonical example of a convex roof measure is the entanglement of formation [BDSW96]. For pure states $|\psi_{AB}\rangle$, it is defined as the von Neumann entropy of a subsystem $E_f(\psi_{AB}) = S(\psi_A)$. Next we extend the measure to ensembles of pure states through convexity, i.e. $E_f(\{(p_i, \psi_i)\}) = \sum_i p_i E_f(\psi_i)$. For mixed states, we take infimum over all ensembles that produce the given mixed state, $E_f(\rho) = \inf_{\sum_i p_i \psi_i = \rho} E_f(\{(p_i, \psi_i)\})$. It is clear that entanglement of formation gives an upper bound on the entanglement cost, as the optimum decomposition is a particular way of preparing the state through LOCC.

Some convex roof measures can be related to other classes of measures. For example, Ref. [SKB10] showed that the convex roof of the geometric measure of entanglement is related to the Bures' distance to separable states.

2.2.3 Distance-based measures

The idea of measuring correlations by distances was proposed in Ref. [VPRK97], which develops a related idea in quantum optics [Hil87]. The authors defined an entanglement measure—relative entropy of entanglement—by taking the relative entropy to the set of separable states, and showed that it is monotonic under LOCC. Although relative entropy is not a metric, it has operational meaning in hypothesis testing that translates to bounds on the rate of several information processing tasks.

More generally, the idea is the following—we take a contractive distance on the set of states and define the measure by simply taking the distance to the set of free states

$$Q(\rho) = \inf_{\sigma \in \mathcal{S}} d(\rho, \sigma). \tag{2.4}$$

By contractive we mean that for any CPTP map φ and any states ρ, σ, we have $d(\varphi(\rho), \varphi(\sigma)) \leq d(\rho, \sigma)$. Since the distance is contractive, it is easy to verify that the constructed measure is a monotone. Furthermore, $Q(\rho)$ is zero if and only if $\rho \in \mathcal{S}$, so the resulting measure is faithful. The measure also inherits the operational meaning of the distance whenever it is defined. For example, trace distance between two states $d_{tr}(\rho, \sigma) = \frac{1}{2}\|\rho - \sigma\|_1$ determines the minimum error of distinguishing two states given a single copy as shown by the Helstrom's bound [Hel76]. Then $Q_{tr}(\rho) = \inf_{\sigma \in \mathcal{S}} d_{tr}(\rho, \sigma)$ determines the minimum error of distinguishing ρ from a free state. When considering many copies in the asymptotic limit, the analogue of trace distance is the quantum relative entropy as shown by quantum Stein's lemma [HP91, NO00]. Therefore, relative entropy-based measures such as relative entropy of entanglement acquire an operational interpretation as the optimal error rate of asymptotic distinguishability. In fact, relative entropy of entanglement is an upper bound to distillable entanglement by the argument outlined in Ref. [VP98].

Measures constructed in this fashion allow us to compare the relative amount of different kinds of correlation in the same state. If we compare two measures that are constructed from the same distance, then the comparison is meaningful. This is not necessarily true for information theoretic measures or convex roof measures.

2.2.4 Minkowski functional and related measures

Some resource theories that we have encountered admit a convex structure—the set of free states *and* free operations are convex. In this case, we can use techniques from convex analysis to quantify correlations.

In convex analysis, the natural measure of distance to a set is the Minkowski functional (also known as gauge) [Roc70]. Therefore, we can apply the formalism in the previous subsection with the Minkowski functional. By choosing different sets, we obtain many quantities that have been extensively studied in quantum information theory [VW02]: base norms [PV07, Reg17], robustness [VT99], best separable approximation [LS98], etc. Given a subset K, the Minkowski functional measures the minimum amount of scaling such that x is contained in the scaled set rK (see Figure 2.2 for illustration).

Definition 2.6. Let K be a subset of a vector space V. The *Minkowski functional of* K is

$$p_K(x) = \inf_{r>0, x \in rK} r \tag{2.5}$$

By convention, we will take the infimum of the empty set as ∞. These functionals are related to norms on the vector space—given a norm $\|x\|$, the Minkowski functional of the unit ball $B = \{x \mid \|x\| = 1\}$ is equal to the norm, i.e. $p_B(x) = \|x\|$. In the literature, this construction is also known as the base norm [Nag, Reg17].

Now, consider the Minkowski functional of the set of free states $p_{\mathcal{S}}$. It is easy to show that $p_{\mathcal{S}}$ is a resource monotone, because free operations preserve the free states.

Robustness [VT99] is defined as $R(\rho) = \inf\{s \mid s \geq 0, \frac{1}{1+s}(\rho + s\sigma) \in SEP, \sigma \in SEP\}$. We can relate robustness to the Minkowski functional of a suitable set [VW02].

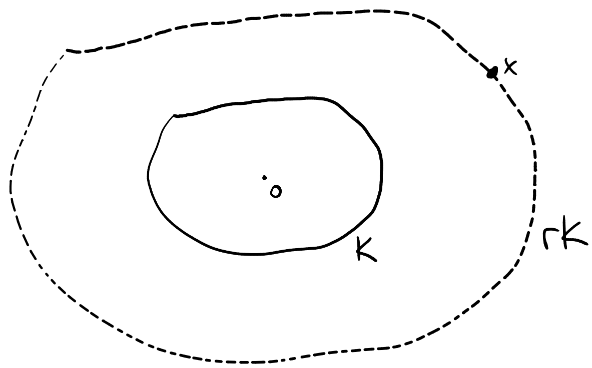

Figure 2.2: Geometrical illustration of the Minkowski functional $p_K(x)$. By considering different subsets K, we recover various correlation measures considered in the literature, including robustness and best separable approximation.

Proposition 2.1. *Let K be the Minkowski difference between separable states, i.e. $K = \{\sigma - \sigma' \mid \sigma, \sigma' \in SEP\}$. Then $R(\rho) = (p_K(\rho) - 1)/2$.*

Proof. Since K is convex, by the Krein-Milman theorem it must be generated by the convex hull of its extreme points [Rud91]. Using the fact $\operatorname{Tr}\rho = 1$, we have

$$p_K(\rho) = \inf\{s \mid \rho = s(a\sigma + b(-\sigma')), a+b=1, a,b \geq 0, \sigma,\sigma' \in SEP\} \tag{2.6}$$
$$= \inf\{a+b \mid \rho = a\sigma - b\sigma', a,b \geq 0, \sigma,\sigma' \in SEP\}. \tag{2.7}$$
$$= \inf\{2s+1 \mid \rho = (1+s)\sigma - s\sigma', \sigma,\sigma' \in SEP\} \tag{2.8}$$
$$= 2R(\rho) + 1 \tag{2.9}$$

Simple rearrangement proves the claim. □

The measure obtained from the best separable approximation has a related construction [LS98]. The measure is defined as $E_{bsa}(\rho) = \inf\{1-p \mid 0 \leq p \leq 1, \rho - p\sigma \geq 0, \sigma \in SEP\}$. It is related to the Minkowski functional as follows [Reg17]:

Proposition 2.2. *Let K be the Minkowski sum $K = \{\frac{1}{2}\sigma + \sigma' \mid \sigma \in \mathcal{D}, \sigma' \in SEP\}$. Then $E_{bsa}(\rho) = p_K(\rho) - 1$.*

Proof. Using the fact that K is convex and $\operatorname{Tr}\rho = 1$, we have

$$p_K(\rho) = \inf\left\{s \mid \rho = s(a\tfrac{1}{2}\sigma + b\sigma'), a+b=1, a,b \geq 0, \sigma \in \mathcal{D}, \sigma' \in SEP\right\} \tag{2.10}$$
$$= \inf\{2a+b \mid \rho = a\sigma + b\sigma', a,b \geq 0, \sigma \in \mathcal{D}, \sigma' \in SEP\} \tag{2.11}$$
$$= \inf\{a+1 \mid \rho = a\sigma + (1-a)\sigma', 0 \leq a \leq 1, \sigma \in \mathcal{D}, \sigma' \in SEP\}. \tag{2.12}$$

Simple rearrangement proves the claim. □

Like distance-based measures, this construction allows us to compare the amount of different types of correlations in a quantum state. For example, we can compare robustness of separability to "robustness of productness" of the same state. However, since they are constructed with tools from convex analysis, they are guaranteed to behave well only for convex theories. This makes it hard to quantify the correlations related to non-convex sets, such as total correlations. As a particular example, let us define the analogue of robustness for total correlations $R_{PROD}(\rho) = (p_K(\rho) - 1)/2$, where we take $K = \{\sigma - \sigma' \mid \sigma, \sigma' \in PROD\}$ to be the Minkowski difference between the set of product states. Note that K is *not* a convex set. Then the following lemma [GMPZ22] implies that the "robustness of productness" $R_{PROD}(\psi) = \infty$ must be infinite for all pure entangled states and hence is not useful as a quantifier of correlations.

Lemma 2.1. *Let ψ be an entangled pure state. Then for any $\chi_A, \chi_B \geq 0, p > 0$,*

$$\rho = p\psi + (1-p)\chi_A \otimes \chi_B \tag{2.13}$$

is not a product state.

Proof. Clearly if $p = 1$, ρ cannot be product because $\rho = \psi$ is entangled. So without loss of generality, we assume that $0 < p < 1$.

We prove by contradiction. Let us assume that ρ can be written as a product $\rho = \rho_A \otimes \rho_B$. Then $\rho_A = p\alpha + (1-p)\chi_A$ and $\rho_B = p\beta + (1-p)\chi_B$, where α and β are the marginals of ψ. Since ψ is entangled, it has at least two terms in the Schmidt decomposition $|\psi\rangle = r_0 |00\rangle + r_1 |11\rangle + \ldots$. Note that in this basis, the reduced states α and β are fully diagonal. We compute the matrix element $\langle 01| \rho |10\rangle$ in two ways: first using $\rho = \rho_A \otimes \rho_B$ and second using the expansion in Eq. (2.13). One finds

$$(1-p)^2 \langle 0| \chi_A |1\rangle \langle 1| \chi_B |0\rangle = \langle 01| \rho |10\rangle = (1-p) \langle 0| \chi_A |1\rangle \langle 1| \chi_B |0\rangle . \tag{2.14}$$

If both local states χ_A and χ_B admit off-diagonal elements, this implies either $p = 0$ or $p = 1$, which contradicts our assumptions. Therefore, at least one of them has to be diagonal in the Schmidt basis. However, a similar computation of the matrix element $\langle 00| \rho |11\rangle$ then implies that $pr_0r_1 = 0$, which contradicts the assumption that ψ is entangled. Therefore for any $p > 0$, ρ is not a product. □

2.3 Computability

The measures presented are generally hard to compute, as most of them involve optimization problems that are hard to solve analytically. Although most of them admit a closed analytical expression for pure states, generally for mixed states they have to be approximated numerically. A notable exception to this is the entanglement of formation for two qubits [HW97], with the formulation of another entanglement monotone called concurrence. Another one is negativity, which is a quantitative version of the PPT separability criterion [Per96, HHH96]. As one of the few entanglement monotones that can be computed for arbitrary mixed state, we will examine negativity and its relation to distance-based measures further in the next chapter.

Recent works have studied various other correlation measures that are computable through semi-definite programming (SDP) [FF18, WW20a, FF21]. Usually they are constructed in the distance-based approach, where the distance measure can be computed through SDP. When the set of uncorrelated states also has an SDP characterization, then we can combine the optimizations into a larger SDP and solve it numerically. Although the solution to the optimization problem remains unsolved analytically, often they are numerically feasible. This also applies to robustness-type measures—if the set of uncorrelated states has an SDP characterization, then the robustness of that correlation is an SDP.

Another property that helps the evaluation of many measures is the convexity of the optimization problem that has to be solved. Convexity makes the optimization much simpler, since any local optimum must be a global optimum. Therefore, to solve such problems, it is enough to use algorithms which guarantee convergence to a local minimum, e.g. gradient descent.

Chapter 3

Partial transpose distance

As one of the few computable entanglement measures, negativity is widely used to characterize the entanglement of an arbitrary state. It originates from Peres' observation that positivity under partial transposition provides a simple necessary but not sufficient condition for entanglement [Per96]. This was later generalized into Horodecki's positive map criterion which is both necessary and sufficient [HHH96]. Even though the partial transpose criterion does not generally detect all entangled state, it is known to be sufficient for two-qubit systems. The equivalence between entanglement and the partial transpose criterion for two-qubit systems implies that the entanglement in PPT states cannot be distilled into Bell pairs [Hor97] and demonstrates a close connection between partial transpose and distillable entanglement.

A quantitative version of Peres' observation was first formulated by Życzkowski et al. [ŻHSL98, Życ99], who called it "degree of entanglement". The name negativity and proof of monotonicity under LOCC operations came later in a paper by Vidal and Werner [VW02]. Negativity is defined as

$$N(\rho_{AB}) = \tfrac{1}{2}(\|T_A(\rho_{AB})\|_1 - 1), \tag{3.1}$$

where $T_A(\rho_{AB})$ denotes the partial transpose of ρ_{AB} in the computational basis of system A. While Peres' criterion checks whether $T_A(\rho_{AB})$ is positive, negativity takes the sum of the negative eigenvalues of $T_A(\rho_{AB})$. There is also a logarithmic version called logarithmic negativity

$$LN(\rho_{AB}) = \log \|T_A(\rho_{AB})\|_1. \tag{3.2}$$

Vidal and Werner also described a connection to base norms, and two operational interpretations of logarithmic negativity: as a lower bound on the singlet distance and upper bound on distillable entanglement. Subsequently, Plenio showed that they are monotonic under a broader set of operations—PPT operations [Ple05].

Generally, negativity provides an easy-to-compute measure of entanglement given the quantum state. We can also understand negativity as a measure derived from Minkowski functional. Let K be the Minkowski difference between partially transposed states, i.e. $K = \{T_A(\sigma - \sigma') \,|\, \sigma, \sigma' \in \mathcal{D}\}$. Then $N(\rho) = \frac{1}{2}(p_K(\rho) - 1)$. Because of this, we can also construct other correlation measures that are comparable to negativity [VW02]. However, this approach has several problems—it is unclear which Minkowski functional should be chosen and it only works if the set of uncorrelated states is convex. Indeed, it will have the same problems that "robustness of productness" suffers from.

In this chapter, we introduce a family of distance-based correlation measures that are related to negativity, i.e. they can be meaningfully compared to negativity. We show that these measures satisfy the usual axioms and provide their operational interpretations. Then we formulate a conjecture for a relation between these measures and negativity, and show cases where this relation holds. We end with a discussion of the geometry of correlations in this distance measure. This chapter is based on Ref. [GMPZ22].

3.1 Introduction

Let us start by motivating a relation between negativity and distance-based measures.

In the quantum information community, there is a widespread belief that coherence and entanglement theory are intimately related. Many of the major ideas in each theory translate well to the other, starting from measures, transformation conditions, existence of golden units, distillation/dilution task, etc. Looking specifically at the resource monotones, we can construct a coherence monotone from a given entanglement measure and vice versa [SSD$^+$15, ZMC$^+$17]. Sometimes, we can even show that there is an analogue of a specific entanglement measure in coherence theory. For example, relative entropy of coherence is closely related to relative entropy of entanglement, as both of them bound distillable coherence/entanglement and coherence/entanglement cost.

Remarkably, negativity also admits such an analogue. Let us start with a correspondence in states between coherence and entanglement theory. To a "coherence theory" state $\rho = \sum_{ij} a_{ij} |i\rangle \langle j|$, we associate an "entanglement theory" state $\tilde{\rho} = \sum_{ij} a_{ij} |ii\rangle \langle jj|$. We can view $\tilde{\rho}$ as mixtures of pure states that have the same Schmidt basis, also known as Schmidt-correlated states. Note that under this correspondence, incoherent states are mapped to separable states—they are even classically-correlated. Ref. [KKS07] showed that the negativity of Schmidt correlated states is equal to the ℓ_1 distance to separable states that are diagonal in the Schmidt basis:

$$N\left(\tilde{\rho} = \sum_{ij} a_{ij} |ii\rangle \langle jj|\right) = \frac{1}{2} \sum_{i \neq j} |a_{ij}| = \inf_{\tilde{\sigma} = \sum_{ij} p_{ij} |ij\rangle \langle ij|} d_{\ell_1}(\tilde{\rho}, \tilde{\sigma}), \tag{3.3}$$

where d_{ℓ_1} is the basis-dependent ℓ_1-distance $d_{\ell_1}(\rho, \sigma) = \frac{1}{2} \sum_{i \neq j} |\langle e_i| (\rho - \sigma) |e_j\rangle|$, computed in the product Schmidt basis. Compare this expression with the ℓ_1-distance coherence measure [BCP14]:

$$C_{\ell_1}\left(\rho = \sum_{ij} a_{ij} |i\rangle \langle j|\right) = \frac{1}{2} \sum_{i \neq j} |a_{ij}| = \inf_{\sigma = \sum_{i} p_{i} |i\rangle \langle i|} d_{\ell_1}(\rho, \sigma), \tag{3.4}$$

where d_{ℓ_1} is computed in the coherence basis. We see that the negativity of $\tilde{\rho}$ is closely related to $C_{\ell_1}(\rho)$. Recent works strengthened this connection by showing that coherence distillation rate is also bounded by C_{ℓ_1}, mirroring the bound on distillable entanglement from logarithmic negativity [RPL16, RPWL17]. When we consider coherence measures that are constructed from entanglement measures [SSD$^+$15], it was shown that C_{ℓ_1} is the measure generated by negativity [ZHC18].

These results suggest that negativity is the image of C_{ℓ_1} under the entanglement-coherence correspondence. In particular, negativity may be related to some distance-based measure, i.e. $N(\rho) = \inf_{\sigma \in S_?} d_?(\rho, \sigma)$ for some distance $d_?$ and set of states $S_?$. Although Refs. [KKS07, NPA13] effectively showed this statement holds for some special states, the distance used was not well-behaved. For example, the distance was basis-dependent, so its value may change if we apply a local unitary to our state. This clearly does not hold for negativity, since it is an entanglement monotone. Therefore, we expect that the distance should also possess similar characteristics to negativity. Since negativity is zero if and only if the state is PPT, this means $S_?$ must be the set of PPT states. Ref. [WW20a] showed that logarithmic negativity can be related to a distance-based measure, where the distance is related to the sandwiched Rényi relative entropy $\tilde{D}_\alpha$:

$$LN(\rho) = \lim_{\alpha\to 1} \inf_{\sigma\in PPT} \frac{\alpha-1}{\alpha} \tilde{D}_\alpha(T_A(\rho) \| T_A(\sigma)), \tag{3.5}$$

$$\tilde{D}_\alpha(X\|Y) = \frac{\alpha}{\alpha-1} \log \left\| Y^{(1-\alpha)/2\alpha} X Y^{(1-\alpha)/2\alpha} \right\|_\alpha, \tag{3.6}$$

where $\|X\|_\alpha = (\mathrm{Tr}\,|X|^\alpha)^{1/\alpha}$ is the Schatten norm of order α. Since the sandwiched Rényi relative is monotonic under CPTP maps [Bei13, MLDS$^+$13, FL13], we can generalize this construction to define measures for other kinds of correlations by replacing the PPT states in the infimum. These measures can be meaningfully compared against logarithmic negativity as they are constructed from the same distance. The problem with this generalization is that the distance to *any* PPT state is constant. This can be seen by noting that for $T_A(\sigma) \geq 0$, we have

$$\lim_{\alpha\to 1} \frac{\alpha-1}{\alpha} \tilde{D}_\alpha(T_A(\rho)\|T_A(\sigma)) = \log \|T_A(\rho)\|_1, \tag{3.7}$$

i.e. the distance is independent of σ. Therefore, it is impossible to distinguish different kinds of correlations with this distance—all of the correlation measures have the same value. Nevertheless, it shows that negativity may be related some distance-based correlation measure.

3.2 Constructing distance from negativity

Let us start by using triangle inequality to relate negativity to a variational expression:

$$\inf_{\sigma\in\mathcal{D}} \tfrac{1}{2}\|T_A(\rho) - \sigma\|_1 \geq \inf_{\sigma\in\mathcal{D}} \tfrac{1}{2}\left(\|T_A(\rho)\|_1 - \|\sigma\|_1\right) = N(\rho). \tag{3.8}$$

Furthermore, if we choose $\sigma^* = \frac{(T_A(\rho))_+}{\mathrm{Tr}\,(T_A(\rho))_+}$, then the inequality is saturated. Therefore, we have

$$N(\rho) = \inf_{\sigma\in\mathcal{D}} \tfrac{1}{2}\|T_A(\rho) - \sigma\|_1, \tag{3.9}$$

capturing the idea that negativity measures how much partially transposed matrix fails to be a state.

Let us define the following distance:

Definition 3.1. The *partial transpose distance* between two bipartite states ρ, σ is defined as

$$d_{T_A}(\rho,\sigma) = \tfrac{1}{2}\left(\|T_A(\rho) - T_A(\sigma)\|_1\right). \tag{3.10}$$

Although partial transposition is a basis-*dependent* map, the partial transpose distance is basis-*independent* because trace norm is invariant under unitaries. Similarly, it does not matter on which subsystem we perform the transposition—only the bipartition matters. When the bipartition is clear from context, we will drop the subscript A for legibility.

Now, Eq. (3.9) can also be written as the partial transpose distance to the set of "partially transposed" density matrices $T_A(\mathcal{D})$, i.e.

$$N(\rho) = \inf_{\sigma\in T_A(\mathcal{D})} \tfrac{1}{2}\|T_A(\rho) - T_A(\sigma)\|_1 = \inf_{\sigma\in T_A(\mathcal{D})} d_T(\rho,\sigma). \tag{3.11}$$

Our main conjecture is this optimum is *always* achieved on the set of PPT states (see Figure 3.1 for illustration).

Conjecture 3.1. *For all states ρ, we have*

$$N(\rho) = \inf_{\sigma\in PPT} d_T(\rho,\sigma). \tag{3.12}$$

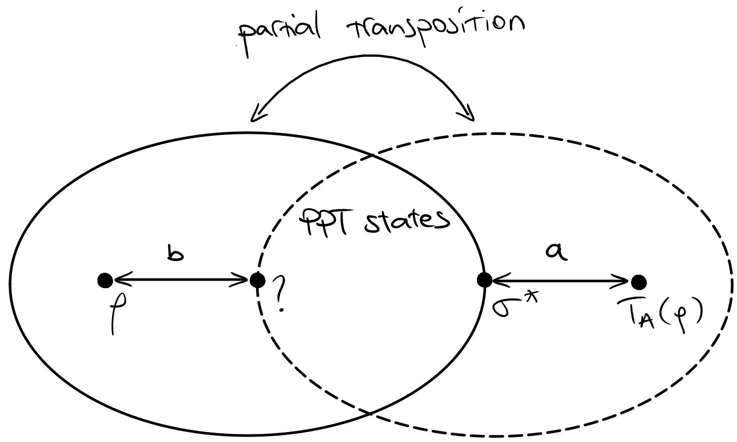

Figure 3.1: Illustration of the conjectured relation between negativity and partial transpose distance (see Conjecture 3.1). The solid line denotes the set of states, and the dashed line denotes the set of partially transposed states. Negativity is equal to the length a, measured through trace distance (see Eq. (3.9)). The state σ^* (see discussion below Eq. (3.8)) achieves this minimum. We conjecture that this length a is always equal to length b, the partial transpose distance to the set of PPT states. Theorem 3.1 shows that the distances are equal when $T_A(\sigma^*)$ is positive semi-definite, i.e. a state. However, in general, the PPT state achieving the minimum partial transpose distance is unknown, as marked by a question mark. We emphasize that this is just an illustration as partial transposition of σ^* can produce matrices with negative eigenvalues, i.e. outside the set of states.

3.3 Evidence for conjecture

We have conjectured that negativity is equal to the partial transpose distance to the set of PPT states. We can prove that this statement holds for a broad class of states that satisfy a particular property.

Definition 3.2. We say the state ρ has *positive binegativity* if $T_A(|T_A(\rho)|) \geq 0$.

Theorem 3.1. *Let ρ be a quantum state that has positive binegativity. Then $N(\rho) = \inf_{\sigma \in PPT} d_T(\rho, \sigma)$.*

Before proving Theorem 3.1, let us note that many states have positive binegativity [ADMVW02, Ish04]. For example, it is known that all pure states, all two-qubit states, two-mode Gaussian states, and Schmidt-correlated states have positive binegativity. Thus, we can understand the results of Ref. [KKS07, NPA13, ZHC18, RPWL17] as showing that Eq. (3.12) holds for particular states. States with positive binegativity are special because we have a closed expression for the exact PPT entanglement cost—that is, how much entanglement is needed to prepare the state with PPT operations in the asymptotic limit. For these states, the cost is exactly logarithmic negativity [APE03, Ish04].

To prove Theorem 3.1, let us start by formulating an alternative form of Conjecture 3.1.

Conjecture 3.2 (alternate form of Conjecture 3.1)**.** *For all states ρ, there exists a PPT state σ such that $(T_A(\rho))_+ \geq \sigma$.*

Proof. We will show that Eq. (3.12) holds if and only if one can find a PPT state σ such that $(T_A(\rho))_+ \geq \sigma$. The proof in one direction is easy—if there is a PPT state σ such that $(T_A(\rho))_+ \geq \sigma$, then we can verify that $d_T(\rho, T_A(\sigma)) = N(\rho)$. Therefore, we only have to show that Eq. (3.12) implies there exists a PPT state σ such that $(T_A(\rho))_+ \geq \sigma$.

Suppose Eq. (3.12) holds, i.e. there exists $\sigma \in PPT$ such that $d_T(\rho, \sigma) = N(\rho)$. Let us choose the optimal σ and show that this implies $(T_A(\rho))_+ \geq T_A(\sigma)$. We have

$$\|T_A(\rho) - T_A(\sigma)\|_1 = 2 d_T(\rho, \sigma) = 2N(\rho) = \|T_A(\rho)\|_1 - \|T_A(\sigma)\|_1. \tag{3.13}$$

Let us write $T_A(\sigma)$ in the blocks corresponding to $(T_A(\rho))_+$ and $(T_A(\rho))_-$, that is $T_A(\sigma) = \begin{pmatrix} X & Z \\ Z^\dagger & Y \end{pmatrix}$, with $X, Y \geq 0$, By using the monotonicity of trace norm under projection onto these diagonal blocks, we have

$$\|T_A(\rho) - T_A(\sigma)\|_1 = \left\| \begin{pmatrix} (T_A(\rho))_+ & 0 \\ 0 & (T_A(\rho))_- \end{pmatrix} - \begin{pmatrix} X & Z \\ Z^\dagger & Y \end{pmatrix} \right\|_1 \tag{3.14}$$

$$\geq \left\| \begin{pmatrix} (T_A(\rho))_+ & 0 \\ 0 & (T_A(\rho))_- \end{pmatrix} - \begin{pmatrix} X & 0 \\ 0 & Y \end{pmatrix} \right\|_1 \tag{3.15}$$

$$= \|(T_A(\rho))_+ - X\|_1 + \|(T_A(\rho))_- - Y\|_1. \tag{3.16}$$

We have reduced the problem to showing that $\|(T_A(\rho))_+ - X\|_1 + \|(T_A(\rho))_- - Y\|_1 = \|T_A(\rho)\|_1 - \|T_A(\sigma)\|_1$ implies $(T_A(\rho))_+ \geq T_A(\sigma)$. Using the inequality $\|A\|_1 \geq \operatorname{Tr} A$ for the first term in Eq. (3.16) and triangle inequality for the second, we have

$$\|(T_A(\rho))_+ - X\|_1 + \|(T_A(\rho))_- - Y\|_1 \geq \operatorname{Tr}((T_A(\rho))_+ - X) + \|(T_A(\rho))_-\|_1 - \|Y\|_1 \tag{3.17}$$

$$= \|T_A(\rho)\|_1 - \|T_A(\sigma)\|_1. \tag{3.18}$$

Because we chose σ such that $\|T_A(\rho) - T_A(\sigma)\|_1 = \|T_A(\rho)\|_1 - \|T_A(\sigma)\|_1$, the inequalities applied to the first and second term must be saturated. Therefore, the following conditions must be satisfied:

1. $\|(T_A(\rho))_+ - X\|_1 = \operatorname{Tr}((T_A(\rho))_+ - X)$, and

2. $\|(T_A(\rho))_- - Y\|_1 = \|(T_A(\rho))_-\|_1 - \|Y\|_1$,

Since $(T_A(\rho))_- - Y \leq 0$, condition 2 implies

$$-\operatorname{Tr}\left((T_A(\rho))_- - Y\right) = \|(T_A(\rho))_- - Y\|_1 \tag{3.19}$$
$$= \|(T_A(\rho))_-\|_1 - \|Y\|_1 = -\operatorname{Tr}(T_A(\rho))_- - \operatorname{Tr} Y, \tag{3.20}$$

i.e. $\operatorname{Tr} Y = 0$. However since $Y \geq 0$, this can only be true if $Y = 0$. Since $Y = 0$ and $T_A(\sigma) = \begin{pmatrix} X & Z \\ Z^\dagger & 0 \end{pmatrix} \geq 0$, we must have $Z = 0$ and $T_A(\sigma) = X$. Therefore condition 1 becomes $\|(T_A(\rho))_+ - T_A(\sigma)\|_1 = \operatorname{Tr}\left((T_A(\rho))_+ - T_A(\sigma)\right)$, which holds true if and only if $(T_A(\rho))_+ \geq T_A(\sigma)$. □

Now, the proof of Theorem 3.1 is immediate.

Proof of Theorem 3.1. Since ρ is a state with positive binegativity, then $T_A((T_A(\rho))_+) \geq 0$. It is easy to verify $\sigma = \frac{1}{\operatorname{Tr}(T_A(\rho))_+}(T_A(\rho))_+$ satisfies the condition given in Conjecture 3.2. □

Theorem 3.1 does not prove the conjecture is true in general, as there exist states that do not have positive binegativity. A simple example of such a state is given by an equal mixture of $|00\rangle + |01\rangle + |12\rangle$ and $|10\rangle + |21\rangle + |22\rangle$. However, a numerical check still confirms that for this particular state, Eq. (3.12) holds. The numerical check can be performed by noting that the partial transpose distance to the set of PPT states is an SDP problem. Furthermore, the alternate version of the conjecture provides a simpler formulation as an SDP feasibility problem. By solving the SDP problem instance corresponding to a given state, we can verify whether Eq. (3.12) holds. The numerical check was implemented in Python, using PICOS [SS22] as a high-level interface and MOSEK as the solver backend.

Nevertheless, we have shown that for a large class of states whose exact PPT entanglement cost is equal to logarithmic negativity, Eq. (3.12) holds. One might ask whether Eq. (3.12) holds for all states whose exact PPT entanglement cost is related to negativity. The problem of computing exact PPT entanglement cost was recently closed in Ref. [WW20b]. The cost is given by the following quantity, called κ-entanglement:

$$E_\kappa(\rho) = \log\inf\left\{\operatorname{Tr} S \mid S \geq 0, -T_A(S) \leq T_A(\rho) \leq T_A(S)\right\}. \tag{3.21}$$

It was shown that both the lower and upper bound from logarithmic negativity given in Ref. [APE03] are not tight in general, by giving an example of a state whose κ-entanglement is strictly between these bounds. Numerical checks using the same method as explained above for these states confirm that Eq. (3.12) holds for this example.

We have also checked whether Eq. (3.12) holds for mixed states chosen randomly according to the recipe given in Refs. [ZS01, Bra96, Hal98]. We sampled two qudit states with local dimension $d = 2$ to $d = 6$, with 10^6 random mixed states for each dimension. In all cases, we have never observed a counterexample to the conjecture—that is, where the negativity is significantly above the partial transpose distance.

In principle, we can attribute the lack of counterexamples to two things: the set of counterexamples might have zero measure, or the negative eigenvalues of $T_A((T_A(\rho))_+)$ are typically very small. Nonetheless, a simple application of triangle inequality shows that $N(\rho) \leq \inf_{\sigma\in PPT} d_T(\rho,\sigma)$. From the calculations on random states, we found that the difference between negativity and the computed partial transpose distance is typically within 10^{-8}, which reflects the precision of the SDP solver. Thus we conclude that negativity provides a good lower bound to the partial transpose distance for a typical state.

3.4 Properties and operational interpretation

Because the partial transpose distance was constructed in relation to negativity, the distance should be contractive in order to guarantee monotonicity (as discussed in Section 2.2.3). However, the following counterexample shows that this distance is *not* contractive under general CPTP operations. Consider two d-level systems and let $|\psi\rangle = |00\rangle$, $|\varphi\rangle = |01\rangle$, such that $d_T(\psi, \varphi) = 1$. Observe that the distance between $|\Phi\rangle = \frac{1}{\sqrt{d}} \sum_i |ii\rangle$ and $\sigma = \frac{1}{d} \sum_i |ii\rangle \langle ii|$ is $(d-1)/2$. Since ψ and φ are orthogonal, there exists a CPTP map Λ that maps $|\psi\rangle$ to Φ and $|\varphi\rangle$ to σ. Then $d_T(\psi, \varphi) = 1 < (d-1)/2 = d_T(\Lambda(\psi), \Lambda(\varphi))$ for $d > 3$.

This does not pose a problem for monotonicity of negativity, because the partial transpose distance is still contractive under PPT operations.

Proposition 3.1. *For any PPT operation φ and density matrices ρ, σ, we have $d_T(\rho, \sigma) \geq d_T(\varphi(\rho), \varphi(\sigma))$.*

Proof. By the definition of PPT operations, $\rho \mapsto T_A(\varphi(T_A(\rho)))$ is a positive map. Since trace norm is monotonic under positive, trace-preserving maps [Rus94], we have

$$\begin{aligned} d_T(\rho, \sigma) &= \tfrac{1}{2} \|T_A(\rho) - T_A(\sigma)\|_1 && (3.22)\\ &\geq \tfrac{1}{2} \|T_A(\varphi(T_A(T_A(\rho)))) - T_A(\varphi(T_A(T_A(\sigma))))\|_1 && (3.23)\\ &= d_T(\varphi(\rho), \varphi(\sigma)), && (3.24) \end{aligned}$$

proving the claim. □

Since partial transpose distance and trace norm are closely related, we expect that the operational interpretation of these two quantities must also be connected. The operational interpretation of trace distance comes from the task of one-shot distinguishability, in a result commonly known as Helstrom's bound [Hel76]. Suppose we are given one copy of a quantum state out of two known choices ρ, σ that are equally likely. Our task is to guess which state we are given, and we are only allowed to do one POVM measurement on our state. If we associate the POVM element P with guessing ρ and $\mathbb{1} - P$ with guessing σ, the probability of a correct guess is given by

$$\begin{aligned} P_{\text{POVM}} &= \tfrac{1}{2} \left(\operatorname{Tr} P\rho + \operatorname{Tr} (\mathbb{1} - P)\sigma \right) && (3.25)\\ &= \tfrac{1}{2} \left(1 + \operatorname{Tr} P(\rho - \sigma) \right). && (3.26) \end{aligned}$$

Optimizing P over all possible POVM elements, we have the Helstrom's bound $P_{\text{POVM}} \leq \frac{1}{2} \left(1 + d_{tr}(\rho, \sigma)\right)$.

Now, suppose the states that we are given are bipartite, and there are restrictions on the possible measurements that we can perform. If we can only implement LOCC measurements, the optimum probability of success is also a norm, called LOCC distinguishability norm [MWW09]. Since negativity is a monotone in the theory of PPT entanglement, it is more relevant to consider restrictions to PPT POVM's, which are POVM's where all the POVM element are PPT operators.

Then the optimum probability of success in this task is

$$\begin{aligned} P_{\text{PPT}} &\leq \sup \left\{ \tfrac{1}{2} \left(1 + \operatorname{Tr}\left(P(\rho - \sigma)\right)\right) \,|\, 0 \leq P \leq \mathbb{1}, 0 \leq T_A(P) \leq \mathbb{1} \right\} && (3.27)\\ &= \sup \left\{ \tfrac{1}{2} \left(1 + \operatorname{Tr}\left(T_A(P)\, T_A(\rho - \sigma)\right)\right) \,|\, 0 \leq P \leq \mathbb{1}, 0 \leq T_A(P) \leq \mathbb{1} \right\} && (3.28)\\ &\leq \sup \left\{ \tfrac{1}{2} \left(1 + \operatorname{Tr}\left(P\, T_A(\rho - \sigma)\right)\right) \,|\, 0 \leq P \leq \mathbb{1} \right\} && (3.29)\\ &= \tfrac{1}{2} \left(1 + d_T(\rho, \sigma)\right). && (3.30) \end{aligned}$$

Unlike Helstrom's bound, this bound is not always achievable. The maximum partial transpose distance between two bipartite states generally grows linearly with the local dimensions, so for $d_T(\rho, \sigma) > 1$ this bound is trivial. However, if the states ρ, σ are PPT, then $d_T(\rho, \sigma) \leq 1$ and we always get a non-trivial bound.

Since the partial transpose distance provides an upper bound to PPT distinguishability, it also provides an upper bound to the distinguishability under any less powerful operations, e.g. one-way LOCC, two-way LOCC, separable operations, etc. This has relevance for data hiding protocols [TDL01, DLT02, EW02].

3.5 Geometry of correlations

We have related negativity to a correlation measure based on the partial transpose distance and in Conjecture 3.1 we hypothesized they are always equal. Indeed, Theorem 3.1 showed that Eq. (3.12) holds for a large class of states. We have also shown that the partial transpose distance is contractive under PPT operations. Now we can construct distance-based correlation measures that are comparable to negativity.

Definition 3.3. Let ρ be a quantum state. The partial-transpose correlation measure is defined as

$$Q_{\mathcal{S}}(\rho) = \inf_{\sigma \in \mathcal{S}} d_T(\rho, \sigma), \tag{3.31}$$

where $\mathcal{S}$ is the set of uncorrelated states.

In this section we will study the properties of this family of measures, and the geometry of correlations. We will also provide closed forms for some of these measures. When possible, we will compare them to relative-entropy based quantities for intuition.

We know that for pure states, all correlations take the same form—if a pure state has *any* correlation at all, then it must be entangled. Furthermore, any nonclassical correlation in a pure state must be entanglement. When we quantify these correlations using relative entropy, this is reflected by the fact that for a pure state, the minimum distance to the set of separable states is achieved by a classically correlated state:

$$\inf_{\sigma \in SEP} S(\psi \| \sigma) = \inf_{\sigma \in CC} S(\psi \| \sigma). \tag{3.32}$$

In particular, the classically correlated state that is obtained by dephasing the pure state in the Schmidt basis achieves this minimum. The next theorem shows that this statement also holds for partial-transpose based measures

Theorem 3.2. *Let ψ be a pure quantum state. Then $Q_{PPT}(\psi) = Q_{CC}(\psi) = N(\psi)$.*

Proof. Recall that pure states have positive binegativity [ADMVW02] and therefore $N(\psi) = Q_{PPT}(\psi) \leq Q_{CC}(\psi)$. Thus, we only need to show that there is a classically correlated state σ such that $d_T(\psi, \sigma) = N(\psi)$. To this end, we write ψ in its Schmidt basis $|\psi\rangle = \sum_i \sqrt{p_i} |ii\rangle$, and define $\sigma = \sum_i p_i |ii\rangle \langle ii|$. Then

$$d_T(\psi, \sigma) = \frac{1}{2} \| T_A(\psi) - T_A(\sigma) \|_1 \tag{3.33}$$

$$= \frac{1}{2} \left\| \sum_{ij} \sqrt{p_i p_j} |ij\rangle \langle ji| - \sum_i p_i |ii\rangle \langle ii| \right\|_1 \tag{3.34}$$

$$= \frac{1}{2} \left\| \sum_{i \neq j} \sqrt{p_i p_j} |ij\rangle \langle ji| \right\|_1 . \tag{3.35}$$

Notice that the matrix $\sum_{i \neq j} \sqrt{p_i p_j} |ij\rangle \langle ji|$ has eigenvalues $\pm\sqrt{p_i p_j}$ with eigenvectors $|ij\rangle \pm |ji\rangle$, for $i < j$. Thus $d_T(\psi, \sigma) = \sum_{i<j} \sqrt{p_i p_j} = N(\psi)$. □

We have computed the value of nonclassical correlations Q_{CC} for pure states. Thus to have a complete picture of all types of correlations in a pure state, we only need to compute total correlations, i.e. the distance to the set of product states. When we use quantifiers based on relative entropy, this is a simple task since the closest product state is simply given by the product of its marginals. However, this is not necessarily true if we use other distance measures. For example, if we use trace distance based quantities, there are states whose product of marginals does not achieve the minimum distance to product states [AFCA13]. The question now is, what happens for partial transpose distance? The following example shows that the product of marginals might not achieve the minimum distance either.

Consider the two-qubit state $\rho = \frac{1}{2}\left|00\right\rangle\left\langle 00\right| + \frac{1}{2}\left|11\right\rangle\left\langle 11\right|$. The marginals are clearly maximally mixed, and the distance is $d_T\left(\rho, \frac{\mathbb{1}}{4}\right) = 0.5$. However the distance to the state $\chi = \left(\frac{1}{\sqrt{2}}\left|0\right\rangle\left\langle 0\right| + \left(1-\frac{1}{\sqrt{2}}\right)\left|1\right\rangle\left\langle 1\right|\right)^{\otimes 2}$ is given by $d_T(\rho,\chi) = \sqrt{2}-1 < 0.5$. We can show that this χ is indeed the closest product state to ρ.

Theorem 3.3. *Let $\sigma = \sum_i p_i \left|ii\right\rangle\left\langle ii\right|$ be a classically-correlated state, with p_i in non-increasing order. Let $m = \max\left\{n \middle| \sum_{i<n}\sqrt{p_i} \leq 1\right\}$. Then*

$$Q_{PROD}(\sigma) = 1 - \sum_{i<m} p_i - \left(1 - \sum_{i<m}\sqrt{p_i}\right)^2, \tag{3.36}$$

and the closest product state is given by:

$$\chi = \left(\sum_{i<m}\sqrt{p_i}\left|i\right\rangle\left\langle i\right| + \left(1-\sum_{i<m}\sqrt{p_i}\right)\left|m\right\rangle\left\langle m\right|\right)^{\otimes 2}. \tag{3.37}$$

Proof. Note that the state σ is diagonal in the basis $\left|ij\right\rangle$, so it is invariant under the projection $A \mapsto \sum_{ij}\left|ij\right\rangle\left\langle ij\right| A \left|ij\right\rangle\left\langle ij\right|$. Since the projection takes product states to product states, a standard argument using contractivity of the distance shows that the closest product state to σ must also be diagonal in the basis $\left|ij\right\rangle$:

$$\chi = \left(\sum_i r_i\left|i\right\rangle\left\langle i\right|\right) \otimes \left(\sum_j s_j\left|j\right\rangle\left\langle j\right|\right), \tag{3.38}$$

with $r_i, s_j \geq 0$ and $\sum_i r_i = \sum_j s_j = 1$.

We will optimize over χ and show that the minimum is given by Eq. (3.36). We have

$$\left\|\sigma - \chi\right\|_1 = \left\|\sum_i p_i\left|ii\right\rangle\left\langle ii\right| - \sum_{ij} r_i s_j\left|ij\right\rangle\left\langle ij\right|\right\|_1 \tag{3.39}$$

$$= \sum_{ij}\left|p_i\delta_{ij} - r_i s_j\right|. \tag{3.40}$$

Separating out the $i = j$ terms from $i \neq j$, we have

$$\left\|\sigma - \chi\right\|_1 = \sum_i \left|p_i - r_i s_i\right| + \sum_{ij}(1-\delta_{ij}) r_i s_j \tag{3.41}$$

$$= \sum_i \left|p_i - r_i s_i\right| + \sum_i r_i(1-s_i) \tag{3.42}$$

$$= \sum_i \left|p_i - r_i s_i\right| + 1 - \sum_i r_i s_i \tag{3.43}$$

$$= \sum_i \left|p_i - r_i s_i\right| + \sum_i (p_i - r_i s_i). \tag{3.44}$$

Using the identity $|x| + x = \max\{0, 2x\}$, we get

$$\|\sigma - \chi\|_1 = \sum_i \max\{0, 2(p_i - r_i s_i)\}. \tag{3.45}$$

Writing $u_i = (r_i + s_i)/2$, $v_i = (r_i - s_i)/2$, we have

$$\|\sigma - \chi\|_1 = \sum_i \max\{0, 2(p_i - (u_i + v_i)(u_i - v_i))\} \tag{3.46}$$

$$= \sum_i \max\{0, 2(p_i - u_i^2 + v_i^2)\}. \tag{3.47}$$

We now find conditions under which this distance is minimized. Minimization over v_i's gives all $v_i = 0$, i.e. the local states are the same $r_i = s_i = u_i$. Hence

$$Q_{PROD}(\sigma) = \inf_{r_i, s_j} \tfrac{1}{2}\|\sigma - \chi\|_1 \tag{3.48}$$

$$= \inf_{u_i} \sum_i \max\{0, p_i - u_i^2\}. \tag{3.49}$$

We will show that the minimum over u_i is achieved when $\tilde{u}_i = \sqrt{p_i}$ for $i < m$, $\tilde{u}_m = 1 - \sum_{i<m} \sqrt{p_i}$, and zero otherwise. Indeed, suppose at first that for some index i_0, we have $u_{i_0} > \sqrt{p_{i_0}}$. We could then consider another state χ' represented by the coefficients u'_i such that $u'_{i_0} = \sqrt{p_{i_0}}, u'_{j_0} = u_{j_0} + u_{i_0} - \sqrt{p_{i_0}}$, where j_0 is an arbitrary index not equal to i_0, and $u'_i = u_i$ whenever $i_0 \neq i \neq j_0$. Then clearly $\sum_i u'_i = 1$, and $\sum_i \max\{0, p_i - u_i'^2\} < \sum_i \max\{0, p_i - u_i^2\}$. Hence, for a state that minimizes Eq. (3.49), we must have $u_i \leq \sqrt{p_i}$ for all i. The problem of finding the optimal set of coefficients u_i in Eq. (3.49) reduces to maximization of the expression $\sum_i u_i^2$ under the constraints: $0 \leq u_i \leq \sqrt{p_i}$, for all i, and $\sum_i u_i = 1$.

Suppose now that $u_1 < \sqrt{p_1}$. We can assume without loss of generality that $u_1 > u_2$ as otherwise we would swap the two numbers and the new set of coefficients would still satisfy the constraints because p_i's are assumed to be in non-increasing order. Consider a new set u'_i, defined as $u'_1 = u_1 + \varepsilon, u'_2 = u_2 - \varepsilon$, where $0 < \varepsilon < \sqrt{p_1} - u_1$, and $u'_i = u_i$ whenever $i > 2$ (if u'_2 is negative we set $u'_2 = 0$ and choose $u'_3 = u_3 - (\varepsilon - u_2)$ and so on). With this choice $\sum_i (u'_i)^2 > \sum_i u_i^2$. Therefore, in the maximal case we must have $\tilde{u}_1 = \sqrt{p_1}$. By repeating the same argument, $\tilde{u}_i = \sqrt{p_i}$ for all $i < m$. It is now easy to see that the maximum for the sum of the remaining coefficients, $\sum_{i \geq m} u_i^2$, is achieved for $\tilde{u}_m = 1 - \sum_{i \leq m} \sqrt{p_i}$ and $\tilde{u}_i = 0$, for $i > m$.

Thus, Eq. (3.49) becomes

$$Q_{PROD}(\sigma) = p_m - \tilde{u}_m^2 + \sum_{i>m} p_i \tag{3.50}$$

$$= 1 - \sum_{i<m} p_i - \left(1 - \sum_{i<m} \sqrt{p_i}\right)^2, \tag{3.51}$$

which completes the proof. □

Note that the state σ that appears in Theorem 3.3 is exactly the closest classically correlated state to a pure state $|\psi\rangle = \sum_i \sqrt{p_i}\,|ii\rangle$. Now, let us compute the total correlation in a pure state to complete the hierarchy. As we saw earlier, it is not a straightforward task because the closest product state is not necessarily the product of marginals. However, since we are using a distance that satisfies the triangle inequality, it is easy to provide an upper bound. Given a pure state ψ, let us denote the classically correlated state that is obtained by dephasing ψ in its Schmidt basis by σ. Let us also denote the total correlation in ψ by $I_T(\psi)$ and the total correlation in σ by $C_T(\psi)$, because it is the "classical correlations" that is contained in ψ. Then applying triangle inequality gives the following upper bound for the total correlation in ψ:

$$I_T(\psi) \leq N(\psi) + C_T(\psi), \tag{3.52}$$

where we have an analytic expression for all the quantities on the right-hand side. Compare this to the relative entropy analogues [MPS+10], where

$$I(\psi) = E(\psi) + C(\psi). \tag{3.53}$$

Interestingly, we can show that the inequality (3.52) is always strict and a stronger inequality holds, exhibiting the non-trivial geometry of correlations in the partial transpose distance.

Theorem 3.4. *Let ψ be a pure state. Then*

$$I_T(\psi) \leq N(\psi) + \tfrac{1}{2} C_T(\psi). \tag{3.54}$$

If ψ is maximally entangled, then we have equality.

Let us first gather the tools necessary to prove Theorem 3.4. We shall repeatedly use the following proposition to compute the trace norm of 2×2 matrices.

Proposition 3.2. *Suppose A is a 2×2 Hermitian matrix*

$$A = a_0 \mathbb{1} + a_x \sigma_x + a_y \sigma_y + a_z \sigma_z, \tag{3.55}$$

with $a_0, a_x, a_y, a_z \in \mathbb{R}$.

Then $\|A\|_1 = 2 \max\left\{|a_0|, \sqrt{a_x^2 + a_y^2 + a_z^2}\right\}$

We will use the inequality shown in the following lemma.

Lemma 3.1. *Let ψ be a pure state. Let χ_S be a product state that is diagonal in the Schmidt basis of ψ. Then*

$$d_T(\psi, \chi_S) \geq N(\psi) + \tfrac{1}{2} C_T(\psi). \tag{3.56}$$

Proof. Let $|\psi\rangle = \sum_i \sqrt{p_i}\, |ii\rangle$ be the Schmidt decomposition of ψ. Then $\sigma = \sum_i p_i \,|ii\rangle \langle ii|$ is the closest classically-correlated state to ψ (see Theorem 3.2). Let $\chi_S = \sum_{ij} r_i s_j \,|ij\rangle \langle ij|$ be an arbitrary product state that is diagonal in the Schmidt basis of ψ. We will show that the inequality holds by direct computation.

By definition, the partial transpose distance is $d_T(\psi, \chi_S) = \frac{1}{2} \|T_A(\psi) - T_A(\chi_S)\|_1$. Notice that $T_A(\psi)$ and $T_A(\chi_S)$ decompose into blocks $\{\Pi_{ii} = |ii\rangle \langle ii|\}$, $\{\Pi_{ij} = |ij\rangle \langle ij| + |ji\rangle \langle ji|\}_{i<j}$, so we can sum the contribution from each block. For the Π_{ii} blocks, we have

$$\langle ii|\, T_A(\psi) - T_A(\chi_S)\, |ii\rangle = p_i - r_i s_i, \tag{3.57}$$

so their total contribution to the norm is

$$\sum_i \|\Pi_{ii} \left(T_A(\psi) - T_A(\chi_S)\right)\|_1 = \sum_i |p_i - r_i s_i|. \tag{3.58}$$

For the Π_{ij} blocks, we obtain the following 2×2 submatrices

$$\Pi_{ij} \left(T_A(\psi) - T_A(\chi_S)\right) = \begin{pmatrix} -r_i s_j & \sqrt{p_i p_j} \\ \sqrt{p_i p_j} & -r_j s_i \end{pmatrix} \tag{3.59}$$

$$= -\left(\frac{r_i s_j + r_j s_i}{2}\right) \mathbb{1} + \sqrt{p_i p_j}\,\sigma_x - \left(\frac{r_i s_j - r_j s_i}{2}\right) \sigma_z. \tag{3.60}$$

By Proposition 3.2,

$$\|\Pi_{ij}\left(T_A(\psi)-T_A(\chi_S)\right)\|_1 = 2\max\left\{\frac{r_is_j+r_js_i}{2}, \sqrt{p_ip_j+\left(\frac{r_is_j-r_js_i}{2}\right)^2}\right\} \tag{3.61}$$

$$\geq 2\max\left\{\frac{r_is_j+r_js_i}{2}, \sqrt{p_ip_j}\right\}. \tag{3.62}$$

The total norm reads

$$\begin{aligned}\|T_A(\psi)-T_A(\chi_S)\|_1 &= \sum_i \|\Pi_{ii}\left(T_A(\psi)-T_A(\chi_S)\right)\|_1 + \sum_{i<j}\|\Pi_{ij}\left(T_A(\psi)-T_A(\chi_S)\right)\|_1 \\ &\geq \sum_i |p_i - r_is_i| + \sum_{i<j} 2\max\left\{\frac{r_is_j+r_js_i}{2}, \sqrt{p_ip_j}\right\} \\ &= \sum_{ij}\delta_{ij}\left|\sqrt{p_ip_j}-\frac{r_is_j+r_js_i}{2}\right| + \sum_{ij}(1-\delta_{ij})\max\left\{\frac{r_is_j+r_js_i}{2}, \sqrt{p_ip_j}\right\}.\end{aligned} \tag{3.63}$$

Let $c_{ij}=\frac{r_is_j+r_js_i}{2}$. Using the identity $2\max\{a,b\}=|a+b|+|a-b|$ inside the second sum, we have

$$\begin{aligned}\|T_A(\psi)-T_A(\chi)\|_1 &\geq \sum_{ij}\delta_{ij}|c_{ij}-\sqrt{p_ip_j}| + \sum_{ij}(1-\delta_{ij})\left(\frac{c_{ij}+\sqrt{p_ip_j}}{2}+\left|\frac{c_{ij}-\sqrt{p_ip_j}}{2}\right|\right) \\ &= \sum_{ij}(1+\delta_{ij})\left|\frac{c_{ij}-\sqrt{p_ip_j}}{2}\right| + \sum_{ij}(1-\delta_{ij})\left(\frac{c_{ij}+\sqrt{p_ip_j}}{2}\right) \\ &= \sum_{ij}(1+\delta_{ij})\left|\frac{c_{ij}-\sqrt{p_ip_j}}{2}\right| + \frac{1-\sum_i r_is_i}{2} + \frac{\left(\sum_i\sqrt{p_i}\right)^2-1}{2} \\ &= \sum_{ij}\left|\frac{c_{ij}-\sqrt{p_ip_j}}{2}\right| + \sum_i\left|\frac{r_is_i-p_i}{2}\right| + \frac{1-\sum_i r_is_i}{2} + \frac{\left(\sum_i\sqrt{p_i}\right)^2-1}{2}.\end{aligned} \tag{3.64}$$

By direct computation, we have

$$\|T_A(\psi)-T_A(\sigma)\|_1 = \left(\sum_i\sqrt{p_i}\right)^2 - 1, \tag{3.65}$$

$$\|T_A(\sigma)-T_A(\chi_S)\|_1 = \sum_i |r_is_i-p_i| + 1 - \sum_i r_is_i. \tag{3.66}$$

We thus have

$$\begin{aligned}\|T_A(\psi)-T_A(\chi_S)\|_1 \geq{}& \|T_A(\psi)-T_A(\sigma)\|_1 + \tfrac{1}{2}\|T_A(\sigma)-T_A(\chi_S)\|_1 \\ &+ \sum_{ij}\left|\frac{c_{ij}-\sqrt{p_ip_j}}{2}\right| - \frac{\left(\sum_i\sqrt{p_i}\right)^2-1}{2}.\end{aligned} \tag{3.67}$$

In the next step, we show that $\sum_{ij}\left|c_{ij}-\sqrt{p_ip_j}\right| + 1 - \left(\sum_i\sqrt{p_i}\right)^2 \geq 0$. Since $\sum_{ij}c_{ij}=1$, we have

$$\sum_{ij} \left|c_{ij} - \sqrt{p_i p_j}\right| + 1 - \left(\sum_i \sqrt{p_i}\right)^2 = \sum_{ij} \left|c_{ij} - \sqrt{p_i p_j}\right| + \sum_{ij} c_{ij} - \sum_{ij} \sqrt{p_i p_j} \tag{3.68}$$

$$= \sum_{ij} \left|c_{ij} - \sqrt{p_i p_j}\right| + \left(c_{ij} - \sqrt{p_i p_j}\right) \tag{3.69}$$

$$= \sum_{ij} 2 \max\{0, c_{ij} - \sqrt{p_i p_j}\} \tag{3.70}$$

$$\geq 0. \tag{3.71}$$

For any χ_S that is diagonal in the Schmidt basis, we therefore obtain

$$d_T(\psi, \chi_S) \geq d_T(\psi, \sigma) + \tfrac{1}{2} d_T(\sigma, \chi_S). \tag{3.72}$$

In the last step we note that the first term on the right-hand side is equal to $N(\psi)$ and the second term is the upper bound on $C_T(\psi)$ as the state χ_S might not be the closest product state to σ. This completes the proof. □

Now we have the necessary tools to prove Theorem 3.4.

Theorem. *Let ψ be a pure state. Then*

$$I_T(\psi) \leq N(\psi) + \tfrac{1}{2} C_T(\psi).$$

If ψ is maximally entangled, then we have equality.

Proof. Let us write ψ in its Schmidt basis $|\psi\rangle = \sum_i \sqrt{p_i} |ii\rangle$ and let us define

$$\begin{aligned} m &= \max\left\{ n \mid \sum_{i<n} \sqrt{p_i} \leq 1 \right\} \\ \chi &= \left(\sum_{i<m} \sqrt{p_i} |i\rangle \langle i| + \left(1 - \sum_{i<m} \sqrt{p_i}\right) |m\rangle \langle m| \right)^{\otimes 2} \\ \sigma_0 &= \sum_i p_i |ii\rangle \langle ii| . \end{aligned} \tag{3.73}$$

Recall that Theorem 3.2 showed that σ_0 is the closest classically-correlated state to ψ and Theorem 3.3 showed that χ is the closest product state to σ_0. We now prove a strict equality

$$d_T(\psi, \chi) = d_T(\psi, \sigma_0) + \tfrac{1}{2} d_T(\sigma_0, \chi). \tag{3.74}$$

and the final inequality follows by noting that the state χ might not be the closest product state to the pure state ψ.

First, notice that $T_A(\psi)$ decomposes as

$$T_A(\psi) = \sum_i p_i |ii\rangle \langle ii| + \sum_{i \neq j} \sqrt{p_i p_j} |ij\rangle \langle ji| , \tag{3.75}$$

with blocks $\{\Pi_{ii} = |ii\rangle \langle ii|\}$ and $\{\Pi_{ij} = |ij\rangle \langle ij| + |ji\rangle \langle ji|\}_{i<j}$. Furthermore, χ is also diagonal in the basis $\{|ij\rangle\}$, and $T_A(\chi) = \chi$. Thus to compute $\|T_A(\psi) - T_A(\chi)\|_1$, we can compute the contributions from each block, and then sum them all up.

First, we look at the Π_{ii} blocks. We have

$$\langle ii| \left(T_A(\psi) - T_A(\chi)\right) |ii\rangle = p_i - \langle ii| \chi |ii\rangle \tag{3.76}$$

$$= \begin{cases} 0, & \text{for } i < m, \\ p_m - \left(1 - \sum_{i<m} \sqrt{p_i}\right)^2, & \text{for } i = m, \\ p_i, & \text{for } i > m. \end{cases} \tag{3.77}$$

Since $\sqrt{p_m} > 1-\sum_{i<m}\sqrt{p_i} \geq 0$ by the definition of m, we must have $p_m - \left(1-\sum_{i<m}\sqrt{p_i}\right)^2 \geq 0$. So the total contribution to the norm from the Π_{ii} blocks is

$$\sum_i \left\| |ii\rangle\langle ii| \left(T_A(\psi) - T_A(\chi)\right) |ii\rangle\langle ii| \right\|_1 = \sum_{i\geq m} p_i - \left(1 - \sum_{i<m}\sqrt{p_i}\right)^2. \tag{3.78}$$

In the Π_{ij} blocks, we have the following submatrix

$$\Pi_{ij}\left(T_A(\psi) - T_A(\chi)\right) = \begin{pmatrix} -\langle ij|\chi|ij\rangle & \sqrt{p_i p_j} \\ \sqrt{p_i p_j} & -\langle ji|\chi|ji\rangle \end{pmatrix}. \tag{3.79}$$

Since $\langle ij|\chi|ij\rangle$ depends on i, j, we look at each case individually.

- $i < j < m$:
  We have $\langle ij|\chi|ij\rangle = \langle ji|\chi|ji\rangle = \sqrt{p_i p_j}$, and hence $\left\|\Pi_{ij}\left(T_A(\psi) - T_A(\chi)\right)\right\|_1 = 2\sqrt{p_i p_j}$.
- $i < m, j = m$:
  We have $\langle im|\chi|im\rangle = \langle mi|\chi|mi\rangle = \sqrt{p_i}\left(1-\sum_{i<m}\sqrt{p_i}\right)$. The Π_{im} sub-matrix reads

$$\Pi_{im}\left(T_A(\psi) - T_A(\chi)\right) = \begin{pmatrix} -\sqrt{p_i}\left(1-\sum_{i<m}\sqrt{p_i}\right) & \sqrt{p_i p_m} \\ \sqrt{p_i p_m} & -\sqrt{p_i}\left(1-\sum_{i<m}\sqrt{p_i}\right) \end{pmatrix} \tag{3.80}$$

$$= \sqrt{p_i}\begin{pmatrix} -\left(1-\sum_{i<m}\sqrt{p_i}\right) & \sqrt{p_m} \\ \sqrt{p_m} & -\left(1-\sum_{i<m}\sqrt{p_i}\right) \end{pmatrix}. \tag{3.81}$$

  We get $\left\|\Pi_{im}\left(T_A(\psi) - T_A(\chi)\right)\right\|_1 = 2\sqrt{p_i p_m}$.
- $i \leq m, j > m$:
  We have $\langle ij|\chi|ij\rangle = \langle ji|\chi|ji\rangle = 0$. Thus

$$\Pi_{ij}\left(T_A(\psi) - T_A(\chi)\right) = \begin{pmatrix} 0 & \sqrt{p_i p_j} \\ \sqrt{p_i p_j} & 0 \end{pmatrix}, \tag{3.82}$$

  and $\left\|\Pi_{ij}\left(T_A(\psi) - T_A(\chi)\right)\right\|_1 = 2\sqrt{p_i p_j}$.
- $i > m, j > m$:
  We have $\langle ij|\chi|ij\rangle = \langle ji|\chi|ji\rangle = 0$, and $\left\|\Pi_{ij}\left(T_A(\psi) - T_A(\chi)\right)\right\|_1 = 2\sqrt{p_i p_j}$.

Summarizing, in all the cases we have $\left\|\Pi_{ij}\left(T_A(\psi) - T_A(\chi)\right)\right\|_1 = 2\sqrt{p_i p_j}$.

Therefore,

$$\begin{aligned}\left\|T_A(\psi) - T_A(\chi)\right\|_1 &= \sum_i \left\|\Pi_{ii}\left(T_A(\psi) - T_A(\chi)\right)\right\|_1 + \sum_{i<j}\left\|\Pi_{ij}\left(T_A(\psi) - T_A(\chi)\right)\right\|_1 \\ &= \sum_{i\geq m} p_i - \left(1-\sum_{i<m}\sqrt{p_i}\right)^2 + \sum_{i<j} 2\sqrt{p_i p_j} \\ &= 1 - \sum_{i<m} p_i - \left(1-\sum_{i<m}\sqrt{p_i}\right)^2 + \sum_{i<j} 2\sqrt{p_i p_j}. \end{aligned} \tag{3.83}$$

Note that $\sum_{i<j} 2\sqrt{p_i p_j} = 2d_T(\psi, \sigma_0)$ and $1 - \sum_{i<m} p_i - \left(1-\sum_{i<m}\sqrt{p_i}\right)^2 = d_T(\sigma_0, \chi)$. We therefore obtain Eq. (3.74).

To prove equality for maximally entangled states, our strategy is to use the result of Lemma 3.1. It shows that the distance from ψ to a product state diagonal in the Schmidt basis is lower bounded by some combination of negativity and classical correlations in ψ. On the other hand, the theorem shows that the distance from ψ to its closest product state is upper bounded by the same combination of negativity and classical correlations. Accordingly, showing that the closest product state is diagonal in the Schmidt basis proves the anticipated equality.

We proceed as follows. Since ψ is maximally entangled, there exists local unitaries U, V such that $(U \otimes V) |\psi\rangle = |\Phi\rangle$, where $|\Phi\rangle = \sum_i \frac{1}{\sqrt{d}} |ii\rangle$. The partial transpose distance and the set of product states are invariant under local unitaries, so we must have $I_T(\psi) = I_T(\Phi)$. Suppose $\chi = \chi_A \otimes \chi_B$ is the closest product state to Φ. Recall the identity $(\mathbb{1} \otimes A) |\Phi\rangle = (A^T \otimes \mathbb{1}) |\Phi\rangle$. Therefore $(U \otimes U^*) |\Phi\rangle = |\Phi\rangle$ for any unitary U, and we can perform an operation $U \otimes U^*$ that makes $\chi_A = \sum_i a_i |i\rangle \langle i|$ diagonal in the Schmidt basis of Φ. The closest product state written in the Schmidt basis now reads:

$$\chi^{T_B} = \sum_{ijk} a_i b_{jk} |ij\rangle \langle ik| . \tag{3.84}$$

We show a projective map Π that preserves the partial transposition of Φ, dephases the closest product state in the Schmidt basis, and preserves the product structure. The contractivity of trace norm [Rus94] under positive trace-preserving maps then shows that the distance to Φ cannot increase:

$$I_T(\Phi) = \frac{1}{2}||\Phi^{T_B} - \chi^{T_B}||_1 \geq \frac{1}{2}||\Pi(\Phi^{T_B}) - \Pi(\chi^{T_B})||_1 = \frac{1}{2}||\Phi^{T_B} - \Pi(\chi^{T_B})||_1. \tag{3.85}$$

Accordingly, there always exists a product state achieving the minimum distance that is diagonal in the Schmidt basis.

The relevant projectors are as follows: $\Pi_{ii} = |ii\rangle \langle ii|$ and $\Pi_{ij} = |ij\rangle \langle ij| + |ji\rangle \langle ji|$. Indeed the matrix Φ^{T_B} is preserved by this operation whereas the product state remains product and is dephased:

$$\sum_i \Pi_{ii}(\chi^{T_B}) + \sum_{i<j} \Pi_{ij}(\chi^{T_B}) = \left(\sum_i a_i |i\rangle \langle i| \right) \otimes \left(\sum_j b_{jj} |j\rangle \langle j| \right). \tag{3.86}$$

This completes the proof. □

To summarize, we have related negativity to a family of correlation measures constructed from the partial transpose distance. We provided an operational interpretation of this distance as a bound on the optimal probability of success in PPT data hiding. We conjectured that negativity is in fact a member of this family and provide supporting evidence. Then we investigated the geometry of correlations in this family and showed that the structure of the correlations is different from the relative entropy based picture.

Chapter 4

Mediated dynamics

Mediated interactions are ubiquitous in physics. The simplest scenario to consider is when there are only two objects interacting via the mediator. Modeled abstractly, we take three systems that admit an $A - M - B$ interaction scheme. In particular, the systems A and B do not interact directly, but only through M. We assume that all three systems can be described by the quantum theory, i.e. there is a Hilbert space associated for each system.

At this stage, there are already some interesting questions that we can ask—what properties must the mediator have so that we can say that the interaction is quantum? Is there a difference between the quantumness of the state of the mediator and the quantumness of the interactions? Is it possible to infer some quantum properties of the mediator without measuring it? Because these questions are stated on a general level, any answer will be applicable across many fields.

We are interested in these questions primarily because we would like to put restrictions on the possible theories on quantum gravity. But there are also more practical applications of this framework. In particular, let us elaborate on the implications for quantum simulators. A quantum simulator is a quantum system with a sufficient level of control, that we can use it to simulate the dynamics of any other quantum system [Fey82, Llo96]. Generally, such a system consists of many qubits along with a universal set of quantum gates. Since single qubit gates and CNOT are known to be universal [NC09, DiV95], it is common to build simulators where the set of gates consists of single qubit gates and two qubit gates. To simulate a given dynamics, we need to compile the unitary to a sequence of the available gates (see Figure 4.1). Now, suppose we want to simulate a 2-local Hamiltonian $H = \sum_i H_i$, where each H_i acts on at most 2 subsystems. There are many approaches to simulate this on a quantum simulator. A common way is through the use of product formulas—also known as Suzuki-Trotter formula [CST$^+$21]:

$$e^{-itH} = \lim_{n\to\infty} \left(\prod_j e^{-i\frac{t}{n}H_j} \right)^n \tag{4.1}$$

This means we can approximate the full unitary e^{-itH} arbitrarily well if we take enough Trotter steps. When we truncate the formula at a certain number of steps r, then the error is bounded by some function of r. In general, to obtain a simulation error ε, the number of Trotter steps that must be taken scales inversely to ε, i.e. $r = O(\varepsilon^{-1})$. Interestingly, there exists a class of dynamics where this error scaling does not hold—we can always simulate the dynamics exactly using a fixed number of gates. When all the terms in the Hamiltonian commute $[H_i, H_j] = 0$, then the Suzuki-Trotter formula gives

$$e^{-itH} = \prod_j e^{-itH_j}, \tag{4.2}$$

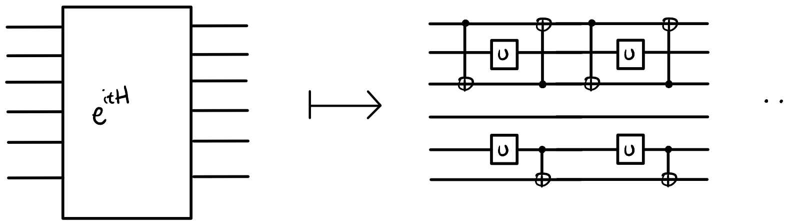

Figure 4.1: Compilation of quantum simulation. The evolution generated by a 2-local Hamiltonian can be compiled to a sequence of one qubit and two qubit gates from a universal gate set through the use of Suzuki-Trotter formula.

i.e. a single Trotter step is sufficient. This means the problem of simulating commuting 2-local Hamiltonians is much simpler than the general problem. By continuity, we expect the error in simulating Hamiltonians that are almost commuting to be small. Indeed, this is what Ref. [CST+21] showed by providing a bound on the asymptotic error in terms of the commutators

$$\varepsilon = O\left(t^2 \sum_{ij} \left\|[H_i, H_j]\right\|_\infty\right). \tag{4.3}$$

Therefore, to obtain a simulation error of at most ε, the number of Trotter steps needed is at least $r = O\left(\varepsilon^{-1} t^2 \sum_{ij} \left\|[H_i, H_j]\right\|_\infty\right)$. We will show that $\sum_{ij} \left\|[H_i, H_j]\right\|_\infty$ is directly linked to the correlations in the system, showing a quantitative relation between the complexity of the simulation and the correlations in the system.

First, we review what was known about mediated systems and what properties can we deduce about an inaccessible mediator. Then we formulate the notion of decomposability, discuss its relation to classicality of interaction as well as its operational interpretation. In addition, we provide a method to witness the nondecomposability of dynamics through the correlation between two probes and define measures of nondecomposability for maps. We outline an experimentally-friendly scheme to provide lower bounds on these nondecomposability measures. This chapter is partially based on Ref. [KGL+18].

4.1 Learning about the mediator

In a sense, the problem of learning about an inaccessible object is everywhere. After all, the goal of physics is to characterize an object and make predictions about its future behavior. Generally, we do this by performing measurements on the system to characterize it, and use our models to predict the future behavior. However, when we say that an object is inaccessible, this implies that we cannot perform measurements on the object. But not all hope is lost—generally the inaccessible object still interacts with other systems. When the inaccessible object does not interact with any other system, then it simply does not matter to our physical models. Therefore, to learn about an inaccessible object, we couple a probe to it, and then perform measurements on the probe. In this way, we can deduce the properties of the inaccessible object. In fact, this is how we model quantum measurements [Pre04, Chapter 3].

Part of the reason of why it is hard to obtain conclusive statements about the quantum features of gravity is because it is not clear what the Hilbert space corresponding to the gravitational field is—perhaps the final theory will not even use Hilbert spaces. We do not have any ways to perform direct measurements on the gravitational system, which rules out

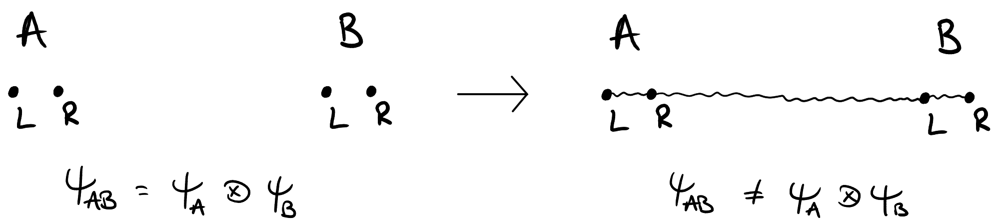

Figure 4.2: The Bose-Marletto-Vedral experiment. Two massive probes A and B are independently prepared in a spatial superposition $|L\rangle + |R\rangle$. The gravitational interaction produces different phases in each component of the superposition, which can be tuned by changing the size of the superposition, the separation between the probes or the interaction time. By tuning these parameters, in principle it is possible to entangle the probes maximally. Left panel: initial configuration. Right panel: the situation at time $t > 0$.

performing any direct Bell tests to see quantum features. Another reason is the magnitude of the gravitational interaction is very small for table-top experiments, practically making detection of gravitational effects very difficult for small quantum objects [Asp22].

Nevertheless, there are several different proposals to witness the nonclassicality of gravity. The famous Colella-Overhauser-Werner (COW) experiment [COW75] confirms that a quantum mechanical system couples to a classical gravitational field $\vec{g} = g\hat{z}$ simply through the potential $V = mgz$. The Bose-Marletto-Vedral (BMV) experiment [BMM$^+$17, MV17] proposed to look at the entanglement between two probes. The idea is the following: we prepare two massive probes, each in a state of spatial superposition (see Figure 4.2). Initially, the joint state of the probes and the gravitational field is in a product state. They argued that if the gravitational field is classical—the joint state of the probes and the gravitational field always has zero discord—then the two probes cannot get entangled. However, when the gravitational interaction is modeled by a quantized Newtonian potential, the two probes do get entangled. Therefore, observation of entanglement between the probes allows us to conclude that gravity has quantum features. In contrast, Ref. [CBPU19] suggests that gravity will induce some decoherence in our probe, which has different spectral characteristic depending on whether the gravitational field is quantum or semiclassical.

At this point, we should draw a distinction between the quantumness of the state of the mediator and the quantumness of the interaction with the mediator. The BMV experiment shows that we can witness the quantumness of the state of the mediator simply by looking at the entanglement between the probes. Recalling the discussion in Chapter 1 (see the discussion before Lemma 1.1), this also means the interaction is classical. However, it is possible that the *state* of the gravitational field is nonclassical, yet the *interaction* is. For example, a quantum state can have non-zero discord, even though the interaction is classical. Concretely, consider the dynamics generated by the Hamiltonian $X_A X_M + X_B X_M$, with the initial state $|\psi_0\rangle = |000\rangle_{ABM}$. At time $t = \pi/4$, the mediator will be entangled with the probes, even though the interaction is completely classical (in the sense of commuting interaction). This distinction raises the question: is it possible to witness the classicality of the interaction instead of the state? How should we even define classical interactions?

In this work, we define the quantumness of interactions through the non-commutativity of the interaction Hamiltonians. As discussed in Chapter 1, we argue that this is a reasonable notion of quantumness for interactions. When we model classical systems by a system with a commuting algebra of observables as in the Koopman-von Neumann formalism [Per02], all classical Hamiltonians will have commuting interaction terms. Therefore, any interaction that has non-commuting terms cannot be simulated by having such a classical mediator.

4.2 Decomposable evolution

Let us start with a closed, tripartite system ABM whose evolution is described by the Hamiltonian $H_{ABM} = H_{AM} + H_{BM}$. We say the interaction is classical if $[H_{AM}, H_{BM}] = 0$, i.e. the interaction terms commute. This implies that the unitary operator $e^{-itH_{ABM}}$ can be decomposed as

$$e^{-itH_{ABM}} = e^{-itH_{AM}} e^{-itH_{BM}} = e^{-itH_{BM}} e^{-itH_{AM}}, \tag{4.4}$$

which can be seen from the Suzuki-Trotter formula. This property of decomposability turns out to be central in witnessing nonclassical interactions.

Definition 4.1. Let U be a unitary acting on a tripartite system $\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_M$. We say U is *decomposable* if there exist unitaries U_{AM}, U_{BM} such that

$$U(\rho_{ABM}) = U_{BM} U_{AM} (\rho_{ABM}). \tag{4.5}$$

Intuitively, decomposable unitaries are those that can be simulated by coupling system A to the mediator M, and then coupling B to the mediator. Although Suzuki-Trotter formula shows that any unitary can be approximated by a sequence of Trotter steps, decomposable unitaries are special because we can implement the exact unitary with only a single Trotter step.

Now let us assume that we have a unitary that is generated by a Hamiltonian $H_{ABM} = H_{AM} + H_{BM}$. Is the classicality of the interaction equivalent to the decomposability of the unitary? The following proposition shows that this is not enough—classical interaction is equivalent to the unitary having a *commuting* decomposition.

Proposition 4.1. *The unitary generated by the Hamiltonian H_{ABM} has a commuting decomposition $e^{iH_{ABM}} = U_{AM}U_{BM} = U_{BM}U_{AM}$ if and only if there exist Hamiltonians H_{AM}, H_{BM} such that $H_{ABM} = H_{AM} + H_{BM}$ and $[H_{AM}, H_{BM}] = 0$.*

Proof. Using the Baker-Campbell-Haussdorf (BCH) [Hal15] formula one easily sees that if such H_{AM}, H_{BM} exists, then $U = e^{iH_{AM}} e^{iH_{BM}} = e^{iH_{BM}} e^{iH_{AM}}$, showing that the unitary has a commuting decomposition.

To show the other direction, suppose the unitary $e^{iH_{ABM}}$ has a commuting decomposition. By definition, there exists U_{AM}, U_{BM} such that $[U_{AM}, U_{BM}] = 0$ and $e^{iH_{ABM}} = U_{AM}U_{BM}$. Let $H_{AM} = -i \log U_{AM}, H_{BM} = -i \log U_{BM}$. Then, these interaction Hamiltonians must commute, because we can write the commutator using the series representation $\log(\mathbb{1} - X) = -\sum_{n=1}^{\infty} \frac{1}{n} X^n$ to get

$$\begin{aligned} [H_{AM}, H_{BM}] &= -[\log U_{AM}, \log U_{BM}] \quad (4.6)\\ &= -\left[\sum_{n=1}^{\infty} \frac{(\mathbb{1} - U_{AM})^n}{n}, \sum_{m=1}^{\infty} \frac{(\mathbb{1} - U_{BM})^m}{m}\right] \quad (4.7)\\ &= 0. \quad (4.8)\end{aligned}$$

Using the BCH formula, we obtain

$$\exp itH_{ABM} = \exp itH_{AM} \exp itH_{BM} = \exp it\,(H_{AM} + H_{BM}). \tag{4.9}$$

Differentiating the expression above with respect to t and using the identity $\frac{d}{dt} \exp(tA)\big|_{t=0} = A$ shows that $H_{ABM} = H_{AM} + H_{BM}$, which proves the claim. □

Therefore, the unitary generated from classical interactions $H_{ABM} = H_{AM} + H_{BM}$ with $[H_{AM}, H_{BM}] = 0$ are decomposable, with the added property that the decomposition must commute $[U_{AM}, U_{BM}] = 0$. Because of this commutation, it does not matter whether we define the decomposition order as $U_{BM}U_{AM}$ or $U_{AM}U_{BM}$. However, in general these orders are not equivalent, as the following proposition shows.

Proposition 4.2. *Let* $U_{AM} = \frac{1}{\sqrt{2}}\left(\mathbb{1} + iZ_A X_M\right)$, $U_{BM} = \frac{1}{\sqrt{2}}\left(\mathbb{1} + iZ_B Z_M\right)$. *Then there are no unitaries* V_{AM}, V_{BM} *such that* $U_{AM}U_{BM} = V_{BM}V_{AM}$.

Proof. We prove by contradiction. Suppose that there exist unitaries V_{AM}, V_{BM} such that $U_{AM}U_{BM} = V_{BM}V_{AM}$. Note that we can write U_{AM}, U_{BM} as

$$U_{AM} = |0\rangle\langle 0|_A \otimes \frac{1}{\sqrt{2}}\left(\mathbb{1}_M + iX_M\right) + |1\rangle\langle 1|_A \otimes \frac{1}{\sqrt{2}}\left(\mathbb{1}_M - iX_M\right), \tag{4.10}$$

$$U_{BM} = |0\rangle\langle 0|_B \otimes \frac{1}{\sqrt{2}}\left(\mathbb{1}_M + iZ_M\right) + |1\rangle\langle 1|_B \otimes \frac{1}{\sqrt{2}}\left(\mathbb{1}_M - iZ_M\right). \tag{4.11}$$

Therefore we have

$$\begin{aligned} U_{AM}U_{BM} = {} & |00\rangle\langle 00|_{AB} \otimes \tfrac{1}{2}\left(\mathbb{1} + iX_M + iY_M + iZ_M\right) \\ & + |01\rangle\langle 01|_{AB} \otimes \tfrac{1}{2}\left(\mathbb{1} + iX_M - iY_M - iZ_M\right) \\ & + |10\rangle\langle 10|_{AB} \otimes \tfrac{1}{2}\left(\mathbb{1} - iX_M - iY_M + iZ_M\right) \\ & + |11\rangle\langle 11|_{AB} \otimes \tfrac{1}{2}\left(\mathbb{1} - iX_M + iY_M - iZ_M\right), \end{aligned} \tag{4.12}$$

i.e. $U_{AM}U_{BM}|ijk\rangle_{ABM} = |ij\rangle_{AB} \otimes |\psi_k\rangle_M$. Observe that we can always write $V_{AM} = \sum_{i,j=0}^{1} |i\rangle\langle j|_A \otimes V_M^{A,ij}$ for some matrices $V_M^{A,ij}$, and similarly for V_{BM}. However, because we assumed $V_{BM}V_{AM} = U_{AM}U_{BM}$, we must have

$$V_{AM} = |0\rangle\langle 0|_A \otimes V_M^{A,0} + |1\rangle\langle 1|_A \otimes V_M^{A,1} \tag{4.13}$$

$$V_{BM} = |0\rangle\langle 0|_B \otimes V_M^{B,0} + |1\rangle\langle 1|_B \otimes V_M^{B,1}, \tag{4.14}$$

where $V_M^{A,0}, V_M^{A,1}, V_M^{B,0}, V_M^{B,1}$ are unitaries on M. This is because if $V_M^{A,10}$ is non-zero, then $V_{BM}V_{AM}|000\rangle_{ABM}$ must have a component along $|1\rangle_A$, which contradicts Eq. (4.12). Therefore, we have

$$\begin{aligned} V_{BM}V_{AM} = {} & |00\rangle\langle 00|_{AB} \otimes V_M^{B,0}V_M^{A,0} \\ & + |01\rangle\langle 01|_{AB} \otimes V_M^{B,1}V_M^{A,0} \\ & + |10\rangle\langle 10|_{AB} \otimes V_M^{B,0}V_M^{A,1} \\ & + |11\rangle\langle 11|_{AB} \otimes V_M^{B,1}V_M^{A,1}. \end{aligned} \tag{4.15}$$

Comparing Eqs. (4.12) and (4.15), we must have

$$V_M^{B,0}V_M^{A,0} = \tfrac{1}{2}\left(\mathbb{1} + iX_M + iY_M + iZ_M\right) \tag{4.16}$$

$$V_M^{B,1}V_M^{A,0} = \tfrac{1}{2}\left(\mathbb{1} + iX_M - iY_M - iZ_M\right) \tag{4.17}$$

$$V_M^{B,0}V_M^{A,1} = \tfrac{1}{2}\left(\mathbb{1} - iX_M - iY_M + iZ_M\right) \tag{4.18}$$

$$V_M^{B,1}V_M^{A,1} = \tfrac{1}{2}\left(\mathbb{1} - iX_M + iY_M - iZ_M\right) \tag{4.19}$$

This leads to

$$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \left(V_M^{B,0}V_M^{A,0}\right)\left(V_M^{B,1}V_M^{A,0}\right)^\dagger \tag{4.20}$$

$$= \left(V_M^{B,0}V_M^{A,1}\right)\left(V_M^{B,1}V_M^{A,1}\right)^\dagger = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \tag{4.21}$$

which is clearly a contradiction. □

Note that Proposition 4.2 also shows that there exists a unitary that is decomposable, yet it is not generated by a classical interaction. Despite this, we will define decomposability in the order $U_{BM}U_{AM}$, keeping in mind that the essential property is decomposable unitaries can be implemented exactly with a single Trotter step.

Does this notion of classicality—or decomposability—restrict the set of possible couplings in any meaningful way? Suppose A and B are same kind of physical system, say both are electrons. Then we expect that they couple to the mediator in the same way. What does it mean for the coupling if the interaction is classical? Well, it is easy to see that if the coupling is of the form $X_A \otimes Y_M + X_B \otimes Y_M$, where $X_{A,B}$ acts on the A, B system and Y_M acts on the mediator, then the interaction terms must commute and the interaction is always classical. As discussed in Chapter 1, such couplings have operator Schmidt rank 1. Therefore, if we witnessed that the interaction cannot be classical, we know that the coupling cannot have operator Schmidt rank 1.

Now, suppose we consider systems that are open to some local environment. In this case, the system does not evolve by some unitary evolution—instead, the evolution of the system is described by a dynamical map $\{\Lambda_t\}_{t\geq 0}$. When the initial state of the system is ρ_0, the state of the system at time t is given by $\rho_t = \Lambda_t(\rho_0)$. To ensure the map is well-behaved, usually we require that for every ρ, the function $t \mapsto \Lambda_t(\rho)$ is continuous, and $\Lambda_0 = \mathbb{1}$. To describe decomposability in this setting, let us generalize the definition of decomposability to quantum maps.

Definition 4.2. Let Λ be a map acting on a tripartite system $\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_M$. We say Λ is *decomposable* if there exist maps $\varphi_{AM}, \varphi_{BM}$, such that

$$\Lambda(\rho_{ABM}) = \varphi_{BM}\varphi_{AM}\left(\rho_{ABM}\right). \tag{4.22}$$

We denote the set of all decomposable maps as `DEC`.

Let us say a few words about the consistency between Definitions 4.1 and 4.2. Clearly, if a unitary is decomposable according to Definition 4.1, then it is also decomposable according to Definition 4.2. The contentious point is the other way around—suppose there exist two maps $\varphi_{AM}, \varphi_{BM}$ such that $U_{ABM} = \varphi_{AM}\varphi_{BM}$. It is not clear a priori that both φ_{AM} and φ_{BM} have to be unitaries. Intuitively, we expect that they must be unitaries because any map that maps any pure state to a pure state, even when acting only on a subsystem, must be unitary. We see this from the Choi state—the Choi state of such a map must be pure, which implies the map is unitary. However, we do not know whether φ_{AM} and φ_{BM} are individually unitaries, so this reasoning is not conclusive. Heuristically, we can also argue that if φ_{AM} is not unitary, then the purity of the output state must be strictly less than that of the input state. But again, this does not constitute a proper proof of the claim, and we will leave this question open. In any case, we will work exclusively with Definition 4.2, and treat the unitary case as a motivating example.

Another point about the consistency of the two definitions—recall that any quantum map has a unitary dilation, also known as Stinespring dilation [NC09]. Is the decomposability of a map Λ equivalent to the decomposability of its unitary dilation? We can show that this holds in at least one direction.

Proposition 4.3. *Let Λ be a decomposable map. Then there exists a Stinespring dilation of Λ*

$$\Lambda(\rho_{ABM}) = \mathrm{Tr}_R\, U_{ABMR}(\rho_{ABM} \otimes \sigma_R)U_{ABMR}^\dagger, \tag{4.23}$$

such that U_{ABMR} is decomposable.

Proof. Because Λ is decomposable, there exist maps $\varphi_{AM}, \varphi_{BM}$ such that $\Lambda = \varphi_{BM}\varphi_{AM}$. The map φ_{AM} must have a Stinespring dilation

$$\varphi_{AM}(\rho_{AM}) = \mathrm{Tr}_{R_A}\, U_{AMR_A}(\rho_{AM} \otimes \sigma_{R_A})U_{AMR_A}^\dagger, \tag{4.24}$$

where R_A is the purifying system for φ_{AM}, Similarly, φ_{BM} must have a dilation with purifying system R_B. Writing the Stinespring dilation for φ_{AM} and φ_{BM}, we get

$$\Lambda(\rho_{ABM}) = \mathrm{Tr}_{R_A R_B} U_{BMR_B} U_{AMR_A} (\rho_{ABM} \otimes \sigma_{R_A} \otimes \sigma_{R_B}) U^\dagger_{AMR_A} U^\dagger_{BMR_B}, \tag{4.25}$$

which proves the claim by identifying $R = R_A R_B$, $U_{ABMR} = U_{BMR_B} U_{AMR_A}$, and $\sigma_R = \sigma_{R_A} \otimes \sigma_{R_B}$. □

We do not know whether decomposability of the Stinespring dilation is also sufficient for decomposability, and we will leave it as an open question.

This notion of decomposability is related to the notion of divisibility in the literature [WC08]. The basic question is the following: given a map Λ, are there quantum maps Λ_1, Λ_2 such that $\Lambda = \Lambda_1 \Lambda_2$? As is, all quantum maps trivially satisfy this property because we can take Λ_1 or Λ_2 to be the identity map. More generally, we can take $\Lambda_1 = \Lambda U$ and $\Lambda_2 = U^\dagger$, where U is any unitary. Therefore, we say Λ is a divisible map if there exists Λ_1, Λ_2 such that $\Lambda = \Lambda_1 \Lambda_2$ and both Λ_1, Λ_2 are not unitaries.

Predating this is the notion of CP-divisibility, studied in the context of Markovian dynamics [Lin76, Gor76, Lid19]. CP-divisibility goes one step further than divisibility—a dynamical map Λ_t is CP-divisible if for any $0 < s < t$, there exists a CP map $V_{t,s}$ such that $\Lambda_t = V_{t,s} \Lambda_s$. Interestingly, the set of CP-divisible maps is not convex [WECC08].

It is worth noting that the divisibility that we consider here has a specific multipartite structure, that was not considered in previous studies. The first work where this multipartite structure arose is in the study of entanglement distribution [SADL15]. It was shown that the maximum entanglement that can be distributed with decomposable maps is bounded by discord in a "virtual" state. We will show that we can generalize this result to detect the nondecomposability of a map, even when we are only given access to some "shadow".

Proposition 4.1 shows that the unitaries generated by classical interactions are a subset of decomposable maps. Therefore, if we can experimentally verify that a given map is not decomposable, we can safely conclude that the interaction is not classical. However, we claimed that we would like to detect it just through the correlations in the probes. To connect these two concepts, we need a notion of "marginals" of decomposable maps, acting only on AB (see Figure 4.3 for illustration).

Definition 4.3. Let $\varphi : \mathcal{D}_A \to \mathcal{D}_{A'}$ be a map. We call $(\tilde{\varphi} : \mathcal{D}_{AR} \to \mathcal{D}_{A'R}, \sigma_R)$ a *dilation* of φ if

$$\varphi(\rho) = \mathrm{Tr}_R\, \tilde{\varphi}(\rho \otimes \sigma_R). \tag{4.26}$$

We denote the set of all dilations of φ as $\mathtt{DIL}(\varphi)$.

Definition 4.4. We say the map $\varphi : AB \to AB$ has a decomposable m-dilation if there exists a dilation $\tilde{\varphi} : ABM \to ABM$ of φ such that $\tilde{\varphi}$ is decomposable and $\dim \mathcal{H}_M \leq m$. We denote the set of all maps with a decomposable m-dilation as $\overline{\mathtt{DEC}}(m)$.

With these definitions, we can state our goal precisely: we wish to infer whether a particular map on AB has *any* decomposable m-dilation, through the correlations generated between AB. If it does not have any decomposable dilation, then the interaction that generates this map must be nonclassical.

4.3 Detection techniques

Using the results from Ref. [SADL15], we can already formulate a scheme to detect whether a map does not have any decomposable m-dilation. The authors showed that given a decomposable map $\varphi = \varphi_{BM} \varphi_{AM}$, the gain in entanglement is bounded by discord

$$E_{A:MB}(\varphi(\rho)) - E_{AM:B}(\rho) \leq D_{AB|M}(\tilde{\rho}), \tag{4.27}$$

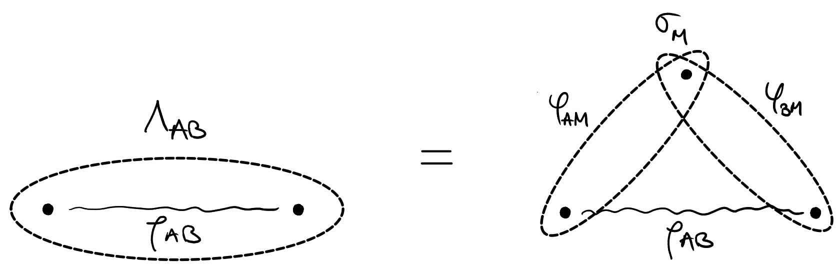

Figure 4.3: Decomposable dilation of a map $\Lambda_{AB}(\rho_{AB})$ into $\mathrm{Tr}_M\, \varphi_{BM}\varphi_{AM}(\rho_{AB}\otimes\sigma_M)$. We provide a witness to detect whether a map has a decomposable dilation with $\dim\mathcal{H}_M \leq m$ by looking at the gain of correlations $Q_{A:B}$. When Λ_{AB} has a decomposable dilation then the maximum output correlation is bounded by the maximum "capacity" of M and a correction from initial correlations (see Corollary 4.1).

where $\tilde{\rho} = \varphi_{AM}(\rho)$ is a so-called virtual state. We say $\tilde{\rho}$ is virtual because it does not represent an actual state in the laboratory, even though it is a proper density matrix. This is because $\tilde{\rho}$ is obtained by applying only the map φ_{AM} to the initial state. Here, discord and entanglement are quantified by distance-based measures constructed from relative entropy. Combining this with the simple bound on the maximum discord, $\log m \geq \sup_\sigma D_{AB|M}(\sigma) \geq D_{AB|M}(\tilde{\rho})$, we get a necessary condition for decomposability: if φ is decomposable, then for any ρ we have

$$E_{A:MB}(\varphi(\rho)) \leq \log m + E_{AM:B}(\rho). \tag{4.28}$$

The condition is most restrictive when $\dim\mathcal{H}_M \leq \dim\mathcal{H}_A \dim\mathcal{H}_B$. In particular, if we choose the initial state to be pure in AB, then it has to be product with M, i.e. $\rho = \psi_{AB}\otimes\sigma_M$. This implies $E_{AM:B}(\psi_{AB}\otimes\sigma_M) = E_{A:B}(\psi_{AB})$, because attaching an uncorrelated subsystem is a reversible local operation. We can also bound the first term by monotonicity, $E_{A:MB}(\varphi(\psi_{AB}\otimes\sigma_M)) \geq E_{A:B}(\mathrm{Tr}_M\,\varphi(\psi_{AB}\otimes\sigma_M))$. Therefore, we can formulate a necessary criterion for decomposable maps, purely in terms of quantities that can be measured on AB: if φ is a decomposable map, then for all ψ_{AB} we have

$$E_{A:B}(\mathrm{Tr}_M\,\varphi(\psi_{AB}\otimes\sigma_M)) \leq \log m + E_{A:B}(\psi_{AB}). \tag{4.29}$$

The key observation is Eq. (4.29) contains only correlations in the subsystems AB. Furthermore, we can ensure that the initial state has the form $\psi_{AB}\otimes\sigma_M$ by preparing a pure state in AB. Therefore, given access only to subsystems AB, we can use violation of Eq. (4.29) to witness when a map cannot have any decomposable m-dilation. As a side remark, note that by a similar reasoning but starting from the results of Ref. [PBK+21], a violation of Eq. (4.29) also detects the presence of discord in the probe-mediator-probe state.

The main result of this chapter is a generalization of this criterion to other continuous correlation quantifiers, as well as a method to estimate measures of nondecomposability. We start by proving a necessary condition for *any* correlation measure assuming the initial state is product.

Theorem 4.1. *Let $\varphi \in$ DEC be a decomposable map. Then for any correlation measure Q, we have*

$$Q_{A:BM}(\varphi(\rho_{AM}\otimes\rho_B)) \leq \sup_{\sigma_{AM}} Q_{A:M}(\sigma_{AM}). \tag{4.30}$$

Proof. Since φ is decomposable, by definition we can find maps $\varphi_{AM}, \varphi_{BM}$ such that $\varphi(\rho_{ABM}) = \varphi_{BM}\varphi_{AM}\,(\rho_{ABM})$. Using the monotonicity of correlations and the definition of decomposability, we have

$$Q_{A:BM}(\varphi\,(\rho_{AM}\otimes\rho_B)) = Q_{A:BM}(\varphi_{BM}\varphi_{AM}\,(\rho_{AM}\otimes\rho_B)) \tag{4.31}$$

$$\leq Q_{A:BM}(\varphi_{AM}\,(\rho_{AM}\otimes\rho_B)). \tag{4.32}$$

Now, note that system B is in a product state with AM. Since Q is a correlation measure, it must be invariant under invertible local operation. In particular, adding or discarding an uncorrelated system must not change the value of Q. Therefore we must have $Q_{A:BM}(\varphi_{AM}(\rho_{AM}\otimes\rho_B)) = Q_{A:M}(\varphi_{AM}(\rho_{AM}))$. Combining this with the bound $Q_{A:M}(\varphi_{AM}(\rho_{AM})) \leq \sup_{\sigma_{AM}} Q_{A:M}(\sigma_{AM})$ finishes the proof. □

Let us see whether this criterion can detect any nondecomposability. For many correlation measures, $\sup_{\sigma_{AM}} Q_{A:M}(\sigma_{AM})$ depends only on the dimension of the smaller Hilbert space. This takes the role of "maximum discord" in Eq. (4.29). For example, it is well-known that for relative entropy of entanglement, $\sup_{\sigma_{AM}} E_{A:M}(\sigma_{AM}) = \log\min\{d_A, d_M\}$. To exhibit an example where bound is violated, let us take $d_A = d_B > d_M$, and Q to be relative entropy of entanglement. The criterion in Theorem 4.1 becomes identical to the bound in Eq. (4.28) if we assume that the initial state is $\rho_{AM}\otimes\rho_B$: for any decomposable map φ, we have

$$E_{A:BM}(\varphi(\rho_{AM}\otimes\rho_B)) \leq \log d_M. \tag{4.33}$$

Now, suppose we take a product state as the initial state $\rho_{ABM} = |000\rangle\langle 000|_{ABM}$ and φ sends it to a maximally entangled state on AB, $\varphi(|000\rangle\langle 000|_{ABM}) = \Phi_{AB}\otimes|0\rangle\langle 0|_M$. We have

$$\log d_A = E_{A:BM}(\varphi(|000\rangle\langle 000|_{ABM})) > \log d_M, \tag{4.34}$$

showing that the maximally entangling map φ cannot be decomposable. However, the criterion does not detect *all* nondecomposable maps, as it becomes trivial when m is large.

To see whether we can witness nondecomposability in a less contrived example, consider a two-level system M acting as a mediator, coupled independently to two cavity light fields A, B acting as probes. We describe the coupling of each field to the mediator by the Jaynes-Cummings model,

$$H_{ABM} = g(a\sigma_+ + a^\dagger\sigma_-) + g(b\sigma_+ + b^\dagger\sigma_-) \tag{4.35}$$

where $a, a^\dagger, b, b^\dagger$ denotes the ladder operator for the fields A, B and $\sigma_\pm$ denotes the raising/lowering operator of the two-level system M. Such models have been studied extensively, both theoretically [Mes02, BP03] and experimentally [RBO$^+$01, HTWR18]. For simplicity, we have assumed the coupling strength of each field to the two-level system is equal. Note that we can write $H_{ABM} = H_{AM} + H_{BM}$ as a sum of two terms: $H_{AM} = g(a\sigma_+ + a^\dagger\sigma_-)$ acting on subsystems A and M, and $H_{BM} = g(b\sigma_+ + b^\dagger\sigma_-)$ acting on subsystems B and M. It is easy to verify that for this decomposition, we have $[H_{AM}, H_{BM}] \neq 0$, showing this interaction might be nonclassical. However, it is not clear a priori that a commuting decomposition of H_{ABM} does not exist—there are infinitely many ways to write H_{ABM} as a sum of two terms. To wit, take $H'_{AM} = H_{AM} + X$ and $H'_{BM} = H_{BM} - X$, where X is an operator acting only on M. Then $H_{ABM} = H'_{AM} + H'_{BM}$ is also a decomposition of H_{ABM} into two terms, each acting only on AM/BM. Theorem 4.1 provides a method to witness the nondecomposability of this Hamiltonian. Combined with Proposition 4.1, this shows that the interaction must be nonclassical. Even more, it is enough to look at the $A:B$ correlation because $Q_{A:B}(\mathrm{Tr}_M\,\varphi(\rho_{AM}\otimes\rho_B)) \leq Q_{A:BM}(\varphi(\rho_{AM}\otimes\rho_B))$.

Figure 4.4 shows the evolution of several correlation measures, defined in Table 4.1. Mutual information and negativity are computed directly, while lower bounds are provided for classical correlation and relative entropy of discord. The classical correlation $C_{A:B}$ is lower bounded by the classical correlation in the computational basis $\tilde{C}_{A:B}$, without the

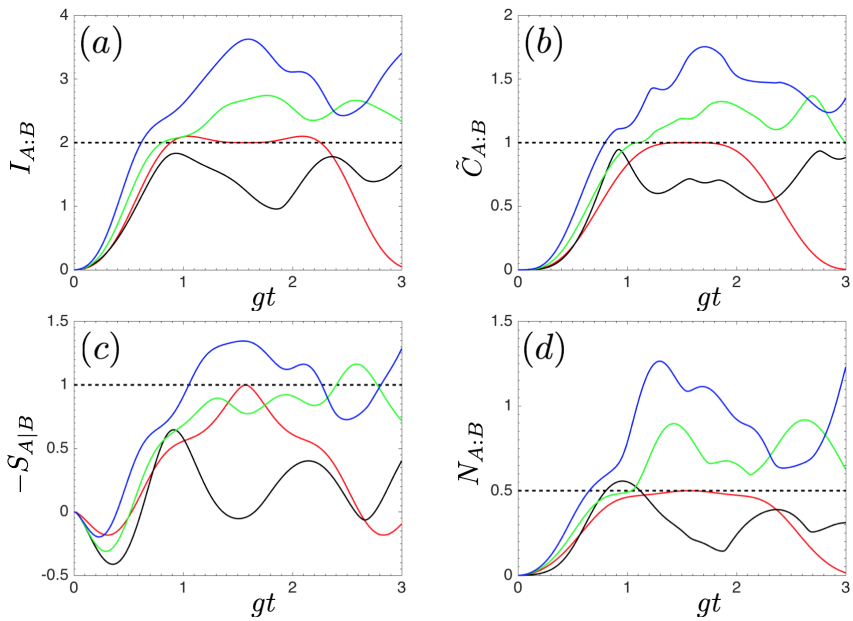

Figure 4.4: Nonclassicality of the Jaynes-Cummings interaction, shown by a violation of the criterion in Theorem 4.1. We simulate the dynamics of several correlation measures (solid curves) and compare them with the corresponding bounds for decomposable evolution (dashed lines). (a) Mutual information, (b) lower bound on the classical correlation (see the main text) (c) lower bound on the relative entropy of discord (see the main text), and (d) negativity. These measures are defined in Table 4.1. In all cases, time is rescaled with the interaction strength g and the initial state of ABM is varied: $|1_A 1_B 0_M\rangle$ (red), $|1_A 0_B 1_M\rangle$ (black), $|2_A 1_B 0_M\rangle$ (green), and $|2_A 2_B 0_M\rangle$ (blue).

Name	Definition	$\sup_{\sigma_{AB}} Q_{A:B}(\sigma_{AB})$
Mutual information	$I_{A:B}(\rho_{AB}) = S(\rho_A) + S(\rho_B) - S(\rho_{AB})$	$2\log\min\{d_A, d_B\}$
Classical correlation	$C_{A:B}(\rho_{AB}) = \sup_{\Pi_A,\Pi_B} I_{A:B}(\Pi_A \otimes \Pi_B(\rho_{AB}))$	$\log\min\{d_A, d_B\}$
Relative entropy of entanglement	$E_{A:B}(\rho_{AB}) = \inf_{\sigma_{AB}\in SEP} S(\rho_{AB}, \sigma_{AB})$	$\log\min\{d_A, d_B\}$
Relative entropy of discord	$D_{B\|A}(\rho_{AB}) = \inf_{\sigma_{AB}\in CQ} S(\rho_{AB}, \sigma_{AB})$	$\log\min\{d_A, d_B\}$
Negativity	$N_{A:B}(\rho_{AB}) = \frac{1}{2}\left(\lVert T_A(\rho_{AB})\rVert_1 - 1\right)$	$\frac{1}{2}\left(\min\{d_A, d_B\} - 1\right)$

Table 4.1: Definitions and maximum values of correlation measures shown in Figure 4.4.

optimization over all bases. For relative entropy of discord $D_{B|A}$, we note the following chain of inequalities: negative conditional entropy $-S_{A|B}(\rho_{AB})$ is a lower bound to distillable entanglement $E_D(\rho_{AB})$ [DW05], which in turn lower bounds the relative entropy of entanglement [HHH00] and the relative entropy of discord:

$$-S_{A|B}(\rho_{AB}) \leq E_D(\rho_{AB}) \leq E_{A:B}(\rho_{AB}) \leq D_{B|A}(\rho_{AB}). \tag{4.36}$$

We observe that if we start with the initial state $|1_A 1_B 0_M\rangle$ (red curves), the nondecomposability is only detected by mutual information, whereas if we start with the initial state $|1_A 0_B 1_M\rangle$ (black curves), it is detected only by negativity. We also note that for the initial states $|2_A 1_B 0_M\rangle$ (green curves) and $|2_A 2_B 0_M\rangle$ (blue curves), we can witness the nondecomposability—and therefore, nonclassicality—of the dynamics even when we only have access to the classical correlations in the probes.

Recall that we discussed whether discord is a form of correlation in Chapter 2. We concluded that it is not, because it can be increased with local operations on the classical subsystem. However, a closer inspection reveals that Theorem 4.1 is applicable to discord, because we only need the correlation measure to be monotonic under all local operations *on one party*. When we apply this to the resource theory of discord and choose system A as the classical side, the argument follows through.

We would like to generalize Theorem 4.1 to allow *any* initial state for the following reason: sometimes in experiments we cannot always perfectly decorrelate two systems—there might be some residual correlations. Therefore, we would like to obtain a statement that is robust to residual correlations. If the correlation measure is continuous, then we expect that continuity will provide some criterion on non-product initial state too. However, there are many variants of continuity—continuity, uniform continuity, asymptotic continuity, etc.—with asymptotic continuity being the most commonly encountered type of continuity in quantum information [Rud64, SRH06]. It is clear that continuity alone is not enough to provide good bounds, as the robustness may depend on which initial state we started with. For a state-independent bound, we need at least uniform continuity. Recall that a function f is called uniformly continuous if for any $\varepsilon > 0$, there exists $\delta(\varepsilon) > 0$ such that for all x, y, $d(x,y) < \delta(\varepsilon)$ implies $|f(x) - f(y)| < \varepsilon$. A function f is called asymptotically continuous if for any sequences $\{\rho_n\}, \{\sigma_n\}$ such that $\|\rho_n - \sigma_n\|_1 \to 0$ as $n \to \infty$, we have $\frac{|f(\rho_n) - f(\sigma_n)|}{\log d_n} \to 0$, where d_n is the dimension of the Hilbert space containing ρ_n, σ_n. This notion of continuity often occurs when considering the asymptotic regime, that is quantities of the form $\frac{1}{n} f(\rho^{\otimes n})$ as $n \to \infty$.

The canonical example of an asymptotically continuous function in quantum information is entropy, shown by the Fannes-Audenaert inequality [Fan73, Aud07].

$$|S(\rho) - S(\sigma)| \leq T \log{(d-1)} + H(\{T, 1-T\}), \tag{4.37}$$

where $T = \frac{1}{2}\|\rho - \sigma\|_1$, d is the dimension of the Hilbert space, and $H(\{p, 1-p\}) = -p \log p - (1-p) \log{(1-p)}$ is the binary entropy function. Many correlation measures considered in the literature are asymptotically continuous. Mutual information is asymptotically continuous as a consequence of Eq. (4.37). Distance-based measures are automatically asymptotically continuous if the distance is bounded. More generally, many relative entropy based measures such as relative entropy of entanglement have also been shown to be asymptotically continuous [DH99], as are convex roof measures that are constructed from asymptotically continuous functions [SRH06]. In fact, these results prove a stronger version of continuity, because they show that there is an *invertible*, monotonically non-decreasing function g such that $|f(x) - f(y)| \leq g(d(x,y))$, and $\lim_{s\to 0} g(s) = 0$.

Definition 4.5. We say f is (g,d)-continuous if there exists a function g such that

$$|f(x) - f(y)| \leq g(d(x,y)) \tag{4.38}$$

for all x, y, where g is invertible, monotonically non-decreasing, and $\lim_{s\to 0} g(s) = 0$.

The results cited above show that many correlation measures are also (g, d)-continuous. It is easy to show that this implies the function f is uniformly continuous—we simply choose $\delta(\varepsilon) = g^{-1}(\varepsilon)$. If the function g is most linear in $\log d_n$, then f is also asymptotically continuous. Any distance-based correlation measure is (g, d)-continuous because of triangle inequality. However, this does not mean that any (g, d)-continuous function is also Lipschitz continuous (or more generally Hölder continuous) for some metric, because $g(d(x, y))$ is not necessarily a proper distance. It is also strictly stronger than uniform continuity. To see this, consider functions on the real line equipped with the discrete metric [Mun00]. Recall the definition of the discrete metric: $d(x, y) = 0$ if and only if $x = y$ and $d(x, y) = 1$ otherwise. With this metric topology, all functions are continuous. However, for a function f to be (g, d)-continuous, we must have $|f(x) - f(y)| < g(d(x, y))$ for some function g, which does not hold if f is unbounded.

For (g, d)-continuous correlation measures where d is a contractive distance, we can prove the following theorem.

Theorem 4.2. *Let $\varphi \in \mathtt{DEC}$ be a decomposable map. Then for any (g, d)-continuous correlation measure Q where d is a contractive distance, we have*

$$Q_{A:BM}(\varphi(\rho_{ABM})) \le \sup_{\sigma_{AM}} Q_{A:M}(\sigma_{AM}) + I_{AM:B}(\rho_{ABM}), \tag{4.39}$$

where $I_{AM:B} = \inf_{\sigma_{AM}\otimes\sigma_B} g(d(\rho_{ABM}, \sigma_{AM} \otimes \sigma_B))$ is a measure of $AM : B$ total correlation in the state ρ_{ABM}.

Proof. Since $Q_{A:BM}$ is (g, d)-continuous, there exists g such that it is invertible, monotonic, $\lim_{s\to 0} g(s) = 0$. Therefore for any $\sigma_{AM} \otimes \sigma_B$, we have

$$\begin{aligned} &|Q_{A:BM}(\varphi(\rho_{ABM})) - Q_{A:BM}(\varphi(\sigma_{AM} \otimes \sigma_B))| \\ &\le g(d(\varphi(\rho_{ABM}), \varphi(\sigma_{AM} \otimes \sigma_B))). \end{aligned} \tag{4.40}$$

Using the monotonicity of g and contractivity of d, we can bound the right-hand side as $g(d(\varphi(\rho_{ABM}), \varphi(\sigma_{AM} \otimes \sigma_B))) \le g(d(\rho_{ABM}, \sigma_{AM} \otimes \sigma_B))$. Combining these two inequalities, rearranging the terms, and taking infimum over all $\sigma_{AM} \otimes \sigma_B$, we get

$$Q_{A:BM}(\varphi(\rho_{ABM})) \le Q_{A:BM}(\varphi(\sigma_{AM} \otimes \sigma_B)) + I_{AM:B}(\rho_{ABM}). \tag{4.41}$$

Finally, we use Theorem 4.1 to bound $Q_{A:BM}(\varphi(\sigma_{AM} \otimes \sigma_B))$, thus proving the claim.

Using of the properties of g and d, it is easy to verify that the quantity $I_{AM:B}(\rho_{ABM}) = \inf_{\sigma_{AM}\otimes\sigma_B} g(d(\rho_{ABM}, \sigma_{AM} \otimes \sigma_B))$ is monotonic under local operations, and it is zero if and only if ρ_{ABM} is product in the bipartition $AM : B$. Therefore, $I_{AM:B}$ is a measure of $AM : B$ total correlation. □

With this, we get the following necessary criterion for maps that have a decomposable m-dilation. This generalizes Eq. (4.29) to *any* continuous correlation measure, at the cost of substituting $E_{A:B}(\psi_{AB})$ with $I_{A:B}(\psi_{AB})$ in the upper bound.

Corollary 4.1. *Let $\varphi \in \overline{\mathtt{DEC}}(m)$ be a map that has a decomposable m-dilation. Then for any (g, d)-continuous correlation measure Q where d is a contractive distance, we have*

$$Q_{A:B}(\varphi(\psi_{AB})) \le \sup_{\sigma_{AM}} Q_{A:M}(\sigma_{AM}) + I_{A:B}(\psi_{AB}), \tag{4.42}$$

where the supremum runs over all $\sigma_{AM} \in \mathcal{D}(\mathcal{H}_A \otimes \mathcal{H}_M)$ with $\dim \mathcal{H}_M \le m$, and $I_{A:B}(\psi_{AB}) = \inf_{\sigma_A\otimes\sigma_B} g(d(\psi_{AB}, \sigma_A \otimes \sigma_B))$ is a measure of $A : B$ total correlation in the state ψ_{AB}.

Proof. Since φ has a decomposable m-dilation, there exist a decomposable map $\tilde{\varphi}$ and a state $\sigma_M \in \mathcal{D}(\mathcal{H}_M)$, such that $\dim \mathcal{H}_M \le m$ and $\varphi(\rho_{AB}) = \mathrm{Tr}_M \tilde{\varphi}(\rho_{AB} \otimes \sigma_M)$. Let us choose the initial state $\rho_{ABM} = \psi_{AB} \otimes \sigma_M$. Applying Theorem 4.2 to $\tilde{\varphi}$, we get

$$Q_{A:BM}(\tilde{\varphi}(\psi_{AB} \otimes \sigma_M)) \le \sup_{\sigma_{AM}} Q_{A:M}(\sigma_{AM}) + I_{AM:B}(\psi_{AB} \otimes \sigma_M). \tag{4.43}$$

Noting that $\mathrm{Tr}_M\,\tilde{\varphi}(\psi_{AB}\otimes\sigma_M)=\varphi(\psi_{AB})$ and $I_{AM:B}(\psi_{AB}\otimes\sigma_M)=I_{A:B}(\psi_{AB})$, we have

$$\begin{aligned} Q_{A:B}(\varphi(\psi_{AB})) &\le Q_{A:BM}(\tilde{\varphi}(\psi_{AB}\otimes\sigma_M)) && (4.44)\\ &\le \sup_{\sigma_{AM}} Q_{A:M}(\sigma_{AM}) + I_{A:B}(\psi_{AB}), && (4.45)\end{aligned}$$

which proves the claim. □

Recalling the example of a violation of the criterion for decomposability in Theorem 4.1, Corollary 4.1 also implies that the maximally entangling map cannot have any decomposable m-dilation when $m<\min\{d_A,d_B\}$. Again, this shows that the criterion in Corollary 4.1 *can* witness that some maps do not have any decomposable m-dilation. Moreover, this can be witnessed with states that are close to product $\rho_{ABM}=\psi_{AB}\otimes\sigma_M\approx\psi_A\otimes\psi_B\otimes\sigma_M$, showing the witness is robust to residual correlations in AB. But similarly to Theorem 4.1, the witness becomes trivial when m is large.

Let us discuss the intuitive origin of such a bound for decomposable evolution. Recall that for any unitary evolution generated by $H_{ABM}=H_{AM}+H_{BM}$, the Suzuki-Trotter formula says that

$$e^{-itH_{ABM}}=\lim_{n\to\infty}\left(e^{-i\frac{t}{n}H_{BM}}e^{-i\frac{t}{n}H_{AM}}\right)^n. \tag{4.46}$$

Thus we can view the evolution as a sequence of discrete exchanges: first A interacts with M for time t/n, and then sends the mediator M over to B. Then B interacts with M and sends the mediator back to A. The evolution is reproduced when we repeat these exchanges $n\to\infty$ times. However, for a decomposable unitary, all of these interactions commute, making the maximum correlation gain equal to the maximum correlation that "M can carry" in a single Trotter step. For a *nondecomposable* unitary, the correlations from each exchange can accumulate, enabling it to go higher than the decomposable bound.

In view of this, we might think that the limitation of dimension of the mediator is arbitrary—a priori, it is completely plausible that all maps have a decomposable dilation if the dimension of the mediator is unbounded. Remarkably, we can show that it is not true—there exists a map that does not have any decomposable dilation, even when we allow the dimension of the mediator to be unbounded.

Proposition 4.4. *The map `SWAP` on two qubits has no decomposable m-dilation for any m.*

Proof. We will prove this by contradiction. Suppose that `SWAP` has a decomposable m-dilation. By definition, there exists two maps $\varphi_{AM},\varphi_{BM}$ and some initial state σ_M such that

$$\begin{aligned} |00\rangle\langle 00|_{AB} &= \mathtt{SWAP}(|00\rangle\langle 00|_{AB}) = \mathrm{Tr}_M\,\varphi_{BM}\varphi_{AM}\left(|00\rangle\langle 00|_{AB}\otimes\sigma_M\right), && (4.47)\\ |10\rangle\langle 10|_{AB} &= \mathtt{SWAP}(|01\rangle\langle 01|_{AB}) = \mathrm{Tr}_M\,\varphi_{BM}\varphi_{AM}\left(|01\rangle\langle 01|_{AB}\otimes\sigma_M\right). && (4.48)\end{aligned}$$

Let us define $\sigma^0_{AM}=\varphi_{AM}\left(|0\rangle\langle 0|_A\otimes\sigma_M\right)$. Now, let us compare the action of `SWAP` on $|00\rangle_{AB}$ and $|01\rangle_{AB}$. By Eqs. (4.47) and (4.48), we have

$$\begin{aligned} |0\rangle\langle 0|_A &= \mathrm{Tr}_B\,\mathtt{SWAP}(|00\rangle\langle 00|_{AB}) = \mathrm{Tr}_{BM}\,\varphi_{BM}\left(|0\rangle\langle 0|_B\otimes\sigma^0_{AM}\right), && (4.49)\\ |1\rangle\langle 1|_A &= \mathrm{Tr}_B\,\mathtt{SWAP}(|01\rangle\langle 01|_{AB}) = \mathrm{Tr}_{BM}\,\varphi_{BM}\left(|1\rangle\langle 1|_B\otimes\sigma^0_{AM}\right). && (4.50)\end{aligned}$$

But φ_{BM} is trace preserving and because Tr_B factors out when applied to product states, we have

$$\begin{aligned} \mathrm{Tr}_{BM}\,\varphi_{BM}\left(|0\rangle\langle 0|_B\otimes\sigma^0_{AM}\right) &= \mathrm{Tr}_{BM}\left(|0\rangle\langle 0|_B\otimes\sigma^0_{AM}\right) && (4.51)\\ &= \mathrm{Tr}_M\,\sigma^0_{AM} && (4.52)\\ &= \mathrm{Tr}_{BM}\,\varphi_{BM}\left(|1\rangle\langle 1|_B\otimes\sigma^0_{AM}\right). && (4.53)\end{aligned}$$

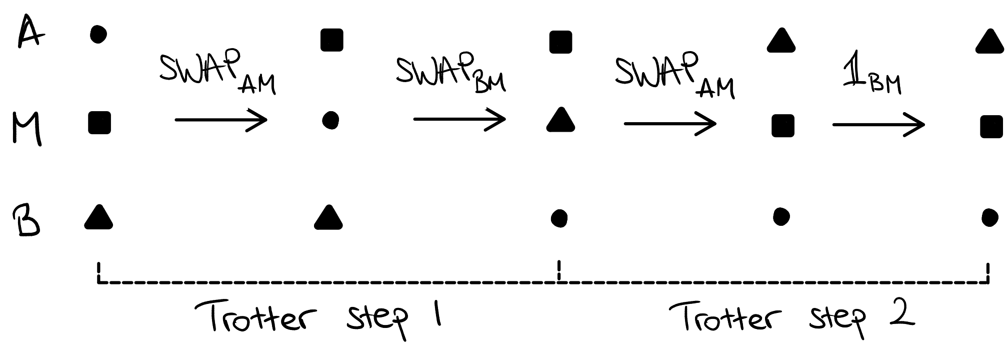

Figure 4.5: An implementation of $\texttt{SWAP}_{AB}$ with two Trotter steps. Proposition 4.4 shows that $\texttt{SWAP}$ does not have any decomposable m-dilation, so it is impossible to implement it with a single Trotter step, even if the mediator M is of infinite dimension. By changing the $\texttt{SWAP}_{BM}$ step, this protocol shows that *any* map can be implemented with two Trotter steps.

Combining this with Eqs. (4.49) and (4.50), we obtain

$$\left|0\right\rangle\left\langle 0\right|_A = \mathrm{Tr}_{BM}\,\varphi_{BM}\left(\left|0\right\rangle\left\langle 0\right|_B \otimes \sigma^0_{AM}\right) \tag{4.54}$$

$$= \mathrm{Tr}_{BM}\,\varphi_{BM}\left(\left|1\right\rangle\left\langle 1\right|_B \otimes \sigma^0_{AM}\right) \tag{4.55}$$

$$= \left|1\right\rangle\left\langle 1\right|_A, \tag{4.56}$$

which is clearly a contradiction. □

This implies the peculiar conclusion that classical interactions *cannot* produce $\texttt{SWAP}$. The intuitive reason behind this statement is it takes at least *two* Trotter steps to implement $\texttt{SWAP}$ with $d_A = d_B = d_M$—first we exchange systems A and M, then we exchange B and M. Finally, we *must* exchange A and M again to complete the implementation (see Figure 4.5). In fact, this protocol shows that *any* map can be implemented with two Trotter steps.

Proposition 4.4 shows that the set of maps that admit a decomposable m-dilation $\bigcup_m \overline{\texttt{DEC}}(m)$ does not include all maps—$\texttt{SWAP}$ is not contained within this set. Clearly, $\overline{\texttt{DEC}}(m)$ forms a nested sequence of sets since $\overline{\texttt{DEC}}(m) \subseteq \overline{\texttt{DEC}}(m+1)$. Furthermore, we can show that all the inclusions are strict. This is because the criterion in Corollary 4.1 can always be saturated for some map in $\overline{\texttt{DEC}}(m)$. Let us fix m and take $d_A = d_B > d_M = m$. Let $\varphi_m(\rho_{AB}) = \mathrm{Tr}_M\,\texttt{SWAP}_{BM}\varphi_{AM}(\rho_{AB} \otimes \left|0\right\rangle\left\langle 0\right|_M)$, where φ_{AM} is a maximally entangling map. By construction, φ_m has a decomposable m-dilation, i.e. $\varphi_m \in \overline{\texttt{DEC}}(m)$. Choosing $\rho_{AB} = \left|00\right\rangle\left\langle 00\right|_{AB}$ and Q to be relative entropy of entanglement, we obtain $E_{A:B}(\varphi_m(\left|00\right\rangle\left\langle 00\right|_{AB})) = \log m$, whereas by Corollary 4.1, for all maps $\varphi \in \overline{\texttt{DEC}}(m-1)$ we must have

$$E_{A:B}(\varphi(\left|00\right\rangle\left\langle 00\right|_{AB})) \leq \sup_{\sigma_{AM}} E_{A:M}(\sigma_{AM}) + I_{A:B}(\left|00\right\rangle\left\langle 00\right|_{AB}) \tag{4.57}$$

$$= \log\,(m-1). \tag{4.58}$$

Therefore $\varphi_m \notin \overline{\texttt{DEC}}(m-1)$, and the inclusion $\overline{\texttt{DEC}}(m) \subsetneq \overline{\texttt{DEC}}(m+1)$ is strict for all m.

4.4 Measures

We have shown how to detect whether a map cannot have any decomposable m-dilation, i.e. $\Lambda \notin \overline{\texttt{DEC}}(m)$. But often, we would like to measure how far it is from any element of $\overline{\texttt{DEC}}(m)$.

For example, a practical motivation would be to bound the error of approximating such a map with an element of $\overline{\texttt{DEC}}(m)$. To this end, let us start by defining a distance measure on maps that is induced by a distance on states.

Definition 4.6. Given two maps $\varphi_1, \varphi_2 : \mathcal{D} \to \mathcal{D}$ and a distance measure on states $d : \mathcal{D} \times \mathcal{D} \to \mathbb{R}$, the *operator distance* is given by

$$d_{op}(\varphi_1, \varphi_2) = \sup_{\sigma \in \mathcal{D}} d(\varphi_1(\sigma), \varphi_2(\sigma)). \tag{4.59}$$

With this, we can already lower bound the distance to $\texttt{DEC}$ based on the violation of the criterion in Theorem 4.2.

Theorem 4.3. *Let Q be a (g, d)-continuous correlation measure, where d is a contractive distance. Let $\Lambda_{ABM} : \mathcal{D}_{ABM} \to \mathcal{D}_{ABM}$ be a map. The distance from Λ_{ABM} to the set $\texttt{DEC}$ is bounded as*

$$\begin{aligned} &\inf_{\varphi_{ABM} \in \texttt{DEC}} d_{op}(\Lambda_{ABM}, \varphi_{ABM}) \\ &\geq \sup_{\rho_{ABM}} g^{-1}\left(Q_{A:BM}(\Lambda_{ABM}(\rho_{ABM})) - \left(\sup_{\sigma_{AM}} Q_{A:M}(\sigma_{AM}) + I_{AM:B}(\rho_{ABM})\right)\right), \end{aligned} \tag{4.60}$$

where $I_{AM:B}(\rho_{ABM}) = \inf_{\sigma_{AM} \otimes \sigma_B} g(d(\rho_{ABM}, \sigma_{AM} \otimes \sigma_B))$ measures the $AM : B$ total correlation in ρ_{ABM}.

Proof. We will prove the theorem by following the steps in the proof of Theorem 4.2, combined with continuity bounds. Let us take a fixed, but arbitrary decomposable map φ_{ABM}. Because of the (g, d)-continuity of $Q_{A:BM}$, we have

$$\begin{aligned} &Q_{A:BM}(\Lambda_{ABM}(\rho_{ABM})) - Q_{A:BM}(\varphi_{ABM}(\rho_{ABM})) \\ &\leq |Q_{A:BM}(\Lambda_{ABM}(\rho_{ABM})) - Q_{A:BM}(\varphi_{ABM}(\rho_{ABM}))| \qquad (4.61) \\ &\leq g(d(\Lambda_{ABM}(\rho_{ABM}), \varphi_{ABM}(\rho_{ABM}))). \qquad (4.62) \end{aligned}$$

Because φ_{ABM} is decomposable, Theorem 4.2 yields

$$Q_{A:BM}(\varphi_{ABM}(\rho_{ABM})) \leq \sup_{\sigma_{AM}} Q_{A:M}(\sigma_{AM}) + I_{AM:B}(\rho_{ABM}), \tag{4.63}$$

where $I_{AM:B}(\rho_{ABM}) = \inf_{\sigma_{AM} \otimes \sigma_B} g(d(\rho_{ABM}, \sigma_{AM} \otimes \sigma_B))$ is a measure of $AM : B$ total correlation. Combining with Eq. (4.62), we get

$$\begin{aligned} &Q_{A:BM}(\Lambda_{ABM}(\rho_{ABM})) - \left(\sup_{\sigma_{AM}} Q_{A:M}(\sigma_{AM}) + I_{AM:B}(\rho_{ABM})\right) \\ &\leq g(d(\Lambda_{ABM}(\rho_{ABM}), \varphi_{ABM}(\rho_{ABM}))). \end{aligned} \tag{4.64}$$

Taking supremum over ρ_{ABM} and using the monotonicity of g, we get

$$\begin{aligned} &\sup_{\rho_{ABM}} Q_{A:BM}(\Lambda_{ABM}(\rho_{ABM})) - \left(\sup_{\sigma_{AM}} Q_{A:M}(\sigma_{AM}) + I_{AM:B}(\rho_{ABM})\right) \\ &\leq g(d_{op}(\Lambda_{ABM}, \varphi_{ABM})). \end{aligned} \tag{4.65}$$

Since φ_{ABM} is an arbitrary decomposable map, we can take the infimum over all decomposable maps $\varphi_{ABM} \in \texttt{DEC}$ to get the tightest bound

$$\begin{aligned} &\sup_{\rho_{ABM}} Q_{A:BM}(\Lambda_{ABM}(\rho_{ABM})) - \left(\sup_{\sigma_{AM}} Q_{A:M}(\sigma_{AM}) + I_{AM:B}(\rho_{ABM})\right) \\ &\leq \inf_{\varphi_{ABM} \in \texttt{DEC}} g(d_{op}(\Lambda_{ABM}, \varphi_{ABM})). \end{aligned} \tag{4.66}$$

Now, since g is monotonic and invertible, g^{-1} must also be monotonic. Applying g^{-1} to both sides of Eq. (4.66) proves the claim. ☐

Since this distance bound is built on the necessary criterion in Theorem 4.2, whenever the criterion is satisfied then the bound on distance must be trivial. Conversely, whenever a violation of the criterion witnesses nondecomposability, Theorem 4.3 will give a non-trivial bound on the distance to decomposable maps. Therefore, the examples given showing the non-triviality of Theorem 4.2 also show the non-triviality of this bound on the distance to decomposable maps.

Let us briefly discuss the implication of this bound to the theory of quantum simulators [CST+21]. Suppose we would like to simulate a unitary, generated by the Hamiltonian $H_{ABM} = H_{AM} + H_{BM}$. We would like to do this by truncating the Suzuki-Trotter formula to r Trotter steps

$$e^{-itH_{ABM}} \approx \left(e^{-i\frac{t}{r}H_{AM}} e^{-i\frac{t}{r}H_{BM}}\right)^r. \tag{4.67}$$

The Suzuki-Trotter formula shows that as $r \to \infty$, this approximation becomes exact. But how do we know when our approximation is good enough? Let us quantify the (additive) error in the simulation by the spectral norm

$$\left\| e^{-itH_{ABM}} - \left(e^{-i\frac{t}{r}H_{AM}} e^{-i\frac{t}{r}H_{BM}}\right)^r \right\|_\infty. \tag{4.68}$$

Ref. [CST+21, Corollary 7] shows that to get the error less than ε, the number of Trotter steps needed scales as the norm of the commutator

$$r = O\left(\frac{t^2}{\varepsilon}\|[H_{AM}, H_{BM}]\|_\infty\right). \tag{4.69}$$

Note that the norm of the commutator $\|[H_{AM}, H_{BM}]\|_\infty$ behaves as a measure of non-decomposability in this bound—the smaller the commutator, the fewer Trotter steps are needed.

Theorem 4.3 relates the correlation in the system to $\inf_{\varphi\in\mathtt{DEC}} d_{op}(e^{-itH_{ABM}}, \varphi)$. Can we relate $\|[H_{AM}, H_{BM}]\|_\infty$ and $\inf_{\varphi\in\mathtt{DEC}} d_{op}(e^{-itH_{ABM}}, \varphi)$? Clearly, when $\|[H_{AM}, H_{BM}]\|_\infty = 0$, then $\inf_{\varphi\in\mathtt{DEC}} d_{op}(e^{-itH_{ABM}}, \varphi) = 0$. We will show a quantitative relation between these two quantities, thus relating the correlations in the system to the number of Trotter steps needed to simulate the dynamics.

Recall that for finite-dimensional systems, *all* metrics generate the same topology [Rud91, Section 1.19], i.e. for any two distances d_1, d_2, there exists a constant C such that

$$\frac{1}{C}d_2(\rho,\sigma) \le d_1(\rho,\sigma) \le C d_2(\rho,\sigma). \tag{4.70}$$

In particular, there exists a constant C relating any distance d to the trace distance $d_{tr}(\rho,\sigma) = \frac{1}{2}\|\rho-\sigma\|_1$. Therefore, if a correlation quantifier on finite dimensional systems is (g,d)-continuous with respect to some distance d, it is also (g,d)-continuous with respect to trace distance. But trace distance is contractive, so Theorem 4.3 applies to any distance d for finite-dimensional systems, at the cost of some constants in g. Now, take the distance derived from the spectral norm $d_\infty(\rho,\sigma) = \|\rho-\sigma\|_\infty$. Ref. [CST+21, Proposition 9] shows that

$$\left\| e^{-it(H_{AM}+H_{BM})} - e^{-itH_{AM}} e^{-itH_{BM}} \right\|_\infty \le \frac{t^2}{2}\|[H_{AM}, H_{BM}]\|_\infty. \tag{4.71}$$

Because $e^{-itH_{AM}} e^{-itH_{BM}}$ is a particular decomposable map, we also have

$$\inf_{\varphi_{ABM}\in\mathtt{DEC}} d_{\infty,op}\left(e^{-itH_{ABM}}, \varphi_{ABM}\right) \le d_{\infty,op}\left(e^{-itH_{ABM}}, e^{-itH_{AM}} e^{-itH_{BM}}\right) \tag{4.72}$$

Therefore the following lemma is sufficient to prove the claim.

Lemma 4.1. *Let U, V be unitaries. Then $d_{\infty,op}(U,V) \le 2\|U-V\|_\infty$.*

Proof. By simple algebra, we easily verify

$$U\rho U^\dagger - V\rho V^\dagger = \tfrac{1}{2}(U-V)\rho(U+V)^\dagger + \tfrac{1}{2}(U+V)\rho(U-V)^\dagger, \tag{4.73}$$

where ρ is a density matrix. Taking the spectral norm on both sides, we get

$$\begin{aligned}\left\|U\rho U^\dagger - V\rho V^\dagger\right\|_\infty &= \left\|\tfrac{1}{2}(U-V)\rho(U+V)^\dagger + \tfrac{1}{2}(U+V)\rho(U-V)^\dagger\right\|_\infty & (4.74)\\ &\le \tfrac{1}{2}\left\|(U-V)\rho(U+V)^\dagger\right\|_\infty + \tfrac{1}{2}\left\|(U+V)\rho(U-V)^\dagger\right\|_\infty & (4.75)\\ &\le \|U-V\|_\infty\|\rho\|_\infty\|U+V\|_\infty & (4.76)\end{aligned}$$

where we used triangle inequality and submultiplicativity of spectral norm $\|AB\|_\infty \le \|A\|_\infty\|B\|_\infty$. Using the bounds $\|\rho\|_\infty \le \|\rho\|_1 = 1$ and $\|U+V\|_\infty \le \|U\|_\infty + \|V\|_\infty = 2$ on the last inequality finishes the proof. □

At this point, Theorem 4.3 is already useful to provide error bounds on the simulation of a general map by decomposable ones. It shows a direct link between correlations and the number of Trotter steps needed—the higher the correlations possible between A and B, the more Trotter steps we need to keep the error small. Note that the analysis above can be extended to simulations of 2-local Hamiltonians on spin chains or many-body systems by considering composite systems as A, B, and M.

This suggests an interesting question: given a unitary U, is the closest element of DEC to U also a unitary? We do not have an answer, but we suspect that the answer highly depends on which distance measure is used.

Recalling the necessary criterion for classical interactions, we would like to extend Theorem 4.3 to bound the distance to $\overline{\texttt{DEC}}(m)$. This is because when we perform experiments, the operationally meaningful quantities should be measurable on AB, whereas Theorem 4.3 provides distances on the ABM operator distance.

Clearly, the ABM operator distance to DEC and the AB operator distance to $\overline{\texttt{DEC}}(m)$ are closely related. Assuming that the distance on states d is contractive to fulfill the assumptions of Theorem 4.3, we have $d_{op}(\Lambda_{ABM}, \varphi_{ABM}) \ge d_{op}(\Lambda_{AB}, \varphi_{AB})$. Therefore, we cannot directly obtain a bound on the operator distance to $\overline{\texttt{DEC}}(m)$, because the inequality is opposite of what we need. To obtain such a bound, let us introduce a completely bounded variant of the operator distance [Pau03].

Definition 4.7. Given two maps $\varphi_1, \varphi_2 : \mathcal{D}_A \to \mathcal{D}_A$ and a distance measure on states $d : \mathcal{D} \times \mathcal{D} \to \mathbb{R}$, the *completely bounded operator distance* is given by

$$d_{cb}(\varphi_1, \varphi_2) = \sup_{\sigma \in \mathcal{D}_{AA'}} d\left(\left(\varphi_1 \otimes \mathbb{1}_{A'}\right)(\sigma), \left(\varphi_2 \otimes \mathbb{1}_{A'}\right)(\sigma)\right), \tag{4.77}$$

where the supremum is taken over all states $\sigma \in \mathcal{D}_{AA'}$, and A' is a finite dimensional Hilbert space with arbitrary dimension.

Proposition 4.5. *Given two maps on finite dimensional systems $\varphi_1, \varphi_2 : \mathcal{D}_A \to \mathcal{D}_B$, we have*

$$d_{cb}(\varphi_1, \varphi_2) = d_{op}(\varphi_1 \otimes \mathbb{1}_{A'}, \varphi_2 \otimes \mathbb{1}_{A'}), \tag{4.78}$$

where the Hilbert space for system A' is finite dimensional with arbitrary dimension.

Proof. Substituting the definition of d_{op} into the definition of d_{cb} proves the claim. □

The benefit of the completely bounded operator distance is it behaves nicely with respect to dilations. This makes it easier to jump from the distance to DEC to the distance to $\overline{\texttt{DEC}}(m)$.

Lemma 4.2. *Let $d : \mathcal{D} \times \mathcal{D} \to \mathbb{R}$ be a contractive distance. Given two maps φ_1, φ_2, we have*

$$d_{cb}(\varphi_1, \varphi_2) = \inf_{\tilde{\varphi}_i \in \texttt{DIL}(\varphi_i)} d_{cb}(\tilde{\varphi}_1, \tilde{\varphi}_2). \tag{4.79}$$

Proof. By contractivity of d, we have $d_{cb}(\varphi_1, \varphi_2) \leq \inf_{\tilde{\varphi}_i \in \mathtt{DIL}(\varphi_i)} d_{cb}(\tilde{\varphi}_1, \tilde{\varphi}_2)$. To show the other direction, we simply observe that $(\tilde{\varphi}_i = \varphi_i \otimes \mathbb{1}, \sigma_i)$ are particular dilations of φ_i, and the claim follows from Proposition 4.5. □

Now we have enough tools to relate Corollary 4.1 to the distance to $\overline{\mathtt{DEC}}(m)$.

Theorem 4.4. *Let Q be a (g, d)-continuous correlation measure, where d is a contractive distance. Let $\Lambda_{AB} : \mathcal{D}_{AB} \to \mathcal{D}_{AB}$ be a map. The distance from Λ_{AB} to the set of maps with a decomposable m-dilation $\overline{\mathtt{DEC}}(m)$ is bounded as*

$$\begin{aligned}
&\inf_{\varphi_{AB} \in \overline{\mathtt{DEC}}(m)} d_{cb}(\Lambda_{AB}, \varphi_{AB}) \\
&\geq \sup_{\psi_{AB}} g^{-1}\left(Q_{A:B}(\Lambda_{AB}(\psi_{AB})) - \left(\sup_{\sigma_{AM}} Q_{A:M}(\sigma_{AM}) + I_{A:B}(\psi_{AB})\right)\right), \qquad (4.80)
\end{aligned}$$

where $I_{A:B}(\psi_{AB})$ measures the $A : B$ total correlation in ψ_{AB}.

Proof. We will essentially continue the proof from Theorem 4.3 and use the completely bounded distance instead of the operator distance.

Let us choose $(\tilde{\Lambda}_{ABM}, \sigma_M)$ as a fixed but arbitrary dilation of Λ_{AB}, and $\tilde{\varphi}_{ABM}$ as a fixed but arbitrary decomposable map. Applying Eq. (4.64) to $\tilde{\Lambda}_{ABM}$ and $\tilde{\varphi}_{ABM}$, we have

$$\begin{aligned}
&d(\tilde{\Lambda}_{ABM}(\rho_{ABM}), \tilde{\varphi}_{ABM}(\rho_{ABM})) \\
&\geq g^{-1}\left(Q_{A:BM}(\tilde{\Lambda}_{ABM}(\rho_{ABM})) - \left(\sup_{\sigma_{AM}} Q_{A:M}(\sigma_{AM}) + I_{AM:B}(\rho_{ABM})\right)\right). \qquad (4.81)
\end{aligned}$$

Now if we take the initial state as a product state that is pure on AB $\rho_{ABM} = \psi_{AB} \otimes \sigma_M$, we have

$$\begin{aligned}
&d(\tilde{\Lambda}_{ABM}(\psi_{AB} \otimes \sigma_M), \tilde{\varphi}_{ABM}(\psi_{AB} \otimes \sigma_M)) \\
&\geq g^{-1}\left(Q_{A:BM}(\tilde{\Lambda}_{ABM}(\psi_{AB} \otimes \sigma_M)) - \left(\sup_{\sigma_{AM}} Q_{A:M}(\sigma_{AM}) + I_{AM:B}(\psi_{AB} \otimes \sigma_M)\right)\right) \qquad (4.82) \\
&\geq g^{-1}\left(Q_{A:B}(\mathrm{Tr}_M \tilde{\Lambda}_{ABM}(\psi_{AB} \otimes \sigma_M)) - \left(\sup_{\sigma_{AM}} Q_{A:M}(\sigma_{AM}) + I_{A:B}(\psi_{AB})\right)\right) \qquad (4.83) \\
&= g^{-1}\left(Q_{A:B}(\Lambda_{AB}(\psi_{AB})) - \left(\sup_{\sigma_{AM}} Q_{A:M}(\sigma_{AM}) + I_{A:B}(\psi_{AB})\right)\right), \qquad (4.84)
\end{aligned}$$

where we use the monotonicity of Q and I under local operations and that $(\tilde{\Lambda}_{ABM}, \sigma_M)$ is a dilation of Λ_{AB}. Taking supremum over initial states ψ_{AB}, we have

$$\begin{aligned}
&\sup_{\psi_{AB}} g^{-1}\left(Q_{A:B}(\Lambda_{AB}(\psi_{AB})) - \left(\sup_{\sigma_{AM}} Q_{A:M}(\sigma_{AM}) + I_{A:B}(\psi_{AB})\right)\right) \\
&\leq \sup_{\psi_{AB}} d(\tilde{\Lambda}_{ABM}(\psi_{AB} \otimes \sigma_M), \tilde{\varphi}_{ABM}(\psi_{AB} \otimes \sigma_M)) \qquad (4.85) \\
&\leq d_{op}(\tilde{\Lambda}_{ABM}, \tilde{\varphi}_{ABM}) \qquad (4.86) \\
&\leq d_{cb}(\tilde{\Lambda}_{ABM}, \tilde{\varphi}_{ABM}). \qquad (4.87)
\end{aligned}$$

Recall that $\tilde{\Lambda}_{ABM}$ is an arbitrary dilation of Λ_{AB}, and $\tilde{\varphi}_{ABM}$ is an arbitrary decomposable map. Since Eq. (4.87) holds for all dilations $\tilde{\Lambda}_{ABM} \in \mathtt{DIL}(\Lambda_{AB})$ and all decomposable maps $\tilde{\varphi}_{ABM} \in \mathtt{DEC}$, we can take infimum to get the tightest bound. Let us define $\varphi_{AB}(\rho_{AB}) = \mathrm{Tr}_M \tilde{\varphi}_{ABM}(\rho_{AB} \otimes \sigma_M)$. By construction, φ_{AB} has a decomposable m-dilation $\tilde{\varphi}_{ABM}$, i.e. $\varphi_{AB} \in \overline{\mathtt{DEC}}(m)$. If we vary $\tilde{\varphi}_{ABM}$ over all decomposable maps, φ_{AB} runs over all maps that admit a decomposable m-dilation. Therefore, taking the infimum and using Lemma 4.2, we get

$$\sup_{\psi_{AB}} g^{-1}\left(Q_{A:B}(\Lambda_{AB}(\psi_{AB})) - \left(\sup_{\sigma_{AM}} Q_{A:M}(\sigma_{AM}) + I_{A:B}(\psi_{AB})\right)\right) \tag{4.88}$$

$$\leq \inf_{\substack{\tilde{\varphi}_{ABM}\in\mathtt{DEC}\\ \tilde{\Lambda}_{ABM}\in\mathtt{DIL}(\Lambda_{AB})}} d_{cb}(\tilde{\Lambda}_{ABM}, \tilde{\varphi}_{ABM}) \tag{4.89}$$

$$= \inf_{\substack{\varphi_{AB}\in\overline{\mathtt{DEC}}(m)\\ \tilde{\varphi}_{ABM}\in\mathtt{DIL}(\varphi_{AB})\\ \tilde{\Lambda}_{ABM}\in\mathtt{DIL}(\Lambda_{AB})}} d_{cb}(\tilde{\Lambda}_{ABM}, \tilde{\varphi}_{ABM}) \tag{4.90}$$

$$= \inf_{\varphi_{AB}\in\overline{\mathtt{DEC}}(m)} d_{cb}(\Lambda_{AB}, \varphi_{AB}), \tag{4.91}$$

which proves the claim. □

A small remark about triviality: similar to the relation between Theorem 4.3 and Theorem 4.2, Theorem 4.4 is built on Corollary 4.1. Since there exist maps that violate the criterion in Corollary 4.1, Theorem 4.4 will provide non-trivial bounds on the distance to $\overline{\mathtt{DEC}}(m)$ for those maps.

Let us discuss the connection between Corollary 4.1, Theorem 4.4, and the BMV experiment. As previously discussed, the BMV experiment shows that the entanglement between the probes AB implies that the joint state ρ_{ABM} of the probes and the mediator must be nonclassical, in the sense of non-zero discord $D_{AB|M}(\rho_{ABM}) > 0$. In contrast to Corollary 4.1, their argument is independent of the dimension of the Hilbert space of the mediator. Is it possible to derive such a criterion from our results? Without any restrictions on the joint state, no such criterion can exist because there is always a decomposable map that saturates the inequality (recall the argument showing that the inclusion $\overline{\mathtt{DEC}}(m) \subsetneq \overline{\mathtt{DEC}}(m+1)$ is strict). Let us examine what happens when we assume that the joint state ABM must always have zero discord $D_{AB|M}(\sigma_{ABM}) = 0$. Using entanglement as our correlation measure, Corollary 4.1 gives

$$E_{A:B}(\varphi(\psi_{AB})) \leq \sup_{\sigma_{AM}} E_{A:M}(\sigma_{AM}) + I_{A:B}(\psi_{AB}), \tag{4.92}$$

for all maps φ that has a decomposable m-dilation, where σ_{AM} runs over all *allowed* joint states of AM. Choosing the initial state $\psi_{AB} = \psi_A \otimes \psi_B$ to be a pure product state, we get

$$E_{A:B}(\varphi(\psi_A \otimes \psi_B)) \leq \sup_{\sigma_{AM}} E_{A:M}(\sigma_{AM}). \tag{4.93}$$

In particular, if we assume that the discord $D_{AB|M}(\sigma_{ABM}) = 0$ must vanish for all allowed joint states σ_{ABM}, we must have $\sup_{\sigma_{AM}} E_{A:M}(\sigma_{AM}) = 0$ and therefore

$$E_{A:B}(\varphi(\psi_A \otimes \psi_B)) \leq 0, \tag{4.94}$$

for all maps φ with a decomposable m-dilation for some m. This is exactly the conclusion of BMV's analysis. However, Eq. (4.93) says much more—if we measured some entanglement between the probes $E_{A:B}(\varphi(\psi_A \otimes \psi_B)) > 0$, and we know that the interaction must be *classical* (and therefore φ has a decomposable dilation), then the $AB : M$ entanglement must be bounded as

$$0 < E_{A:B}(\varphi(\psi_A \otimes \psi_B)) \leq \sup_{\sigma_{AM}} E_{A:M}(\sigma_{AM}) \leq \sup_{\sigma_{ABM}} E_{AB:M}(\sigma_{ABM}) \tag{4.95}$$

where σ_{ABM} runs over the allowed joint states of ABM. So assuming that the interaction is classical, any entanglement between the probes implies that the joint state between the probes and the mediator must be able to carry at least the same amount of entanglement too. In particular, even if we relax the assumption of zero discord $D_{AB|M}(\sigma_{ABM}) = 0$ to zero entanglement, $E_{AB|M}(\sigma_{ABM}) = 0$, the conclusion of the BMV analysis still holds. Another way that our results extend the BMV analysis is we provide quantitative bounds on the nonclassicality of the interaction, through Theorem 4.4.

To summarize, we have defined nonclassicality of mediated interactions through commutativity. We outlined a method to detect the nondecomposability of maps, independently of the actual interactions. The bound generally only depends on the dimension of the mediator, which makes the criterion applicable to situations where the coupling is not sufficiently characterized yet to write down the Hamiltonian. As an application, we related the amount of correlations in the system to the number of Trotter steps needed in a quantum simulator. Furthermore, to provide testable predictions of possible theories of quantum gravity, we also formulated a criterion detecting whether a map can have a decomposable dilation with a mediator with bounded dimension. Finally, we defined measures of nondecomposability of maps and outlined a way to estimate these measures linked to the detection techniques.

Chapter 5

Conclusions

We have discussed various aspects of correlations and their connections to mediated dynamics. Specifically, we formulated a witness of nonclassicality of interactions based on the correlations in two probes. However, many open problems remain.

In Chapter 2, we proposed that correlations are simply a special form of resource theories. We proposed an axiomatic definition to distinguish the typical theories of correlations—entanglement, total correlations, classical correlations, etc.—from general resource theories. Furthermore, we identified correlation measures simply as resource monotones. However, some theories such as discord and Bell nonlocality are left out. Is there a set of "natural" axioms that distinguish theories of correlations from resource theories more generally?

Chapter 3 analyzed the relation between negativity and distance-based correlation measures. In view of suggestive results showing correspondence between coherence theory and entanglement theory, we hypothesized that negativity can be constructed as a distance-based measure. To this end, we conjectured that the partial transpose distance is closely related to negativity (Conjecture 3.1). While we showed that this relation holds in some special cases (see Theorem 3.1), the general case remains an open problem. This conjectured relation allows us to construct distance-based measures for other types of correlation that are comparable to negativity. We presented closed forms of these measures for select cases. Unfortunately, we were unable to obtain a closed formula for the total correlation in pure states. At a more general level, these results suggest that perhaps the correct correspondence is not between coherence theory and entanglement theory, but rather PPT entanglement theory. It seems that further investigation in this direction is needed.

Chapter 4 explored correlations in mediated dynamics, as well as notions of classical interaction. We considered two probe systems whose interactions are relayed through a mediator. We proposed that classical interactions can be defined through commutativity—when the interaction terms in the Hamiltonian commute, then the interaction is classical. In relation to this, we defined decomposability of dynamics and showed that it is a necessary condition for classicality. However, the connection between these two concepts as well as various subtleties regarding the definition of decomposability were not yet fully answered in this thesis. We moved on to formulating a necessary criterion for decomposability in terms of correlations in the probes, independent of the exact coupling to the mediator. While this is primarily the approach taken in this thesis, other alternatives are also worth exploring. We formulated measures of nondecomposability, along with methods of estimation. We related this framework to the theory of quantum simulators, showing a link between correlations and the number of Trotter steps needed in a simulation. In the remaining part of Chapter 4, we extended the analysis to cases where the mediator is inaccessible. We discussed the relation between our results to BMV's analysis and generalized their argument. Namely, not only non-zero entanglement witnesses quantum features of gravity, if we assume the interaction is classical then it also provides a lower bound to the amount of entanglement that the gravitational field can hold. If we do not assume classicality of the interactions, then we obtain a lower bound to the set of classical interactions. The main assumption that we used is that the dimension of the mediator is bounded. Another approach taken in our analysis is in the initial state, the probes are uncorrelated with the mediator, which is enforced by assuming that initially our probes are in a pure state. It would be interesting to extend the analysis to scenarios where there are some initial correlations present.

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