Existence and Uniqueness in the Quantum Marginal Problem

by

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ABSTRACT

EXISTENCE AND UNIQUENESS IN THE QUANTUM MARGINAL PROBLEM

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The quantum marginal problem asks whether a family of quantum marginals are compatible with a global quantum state. It is of central importance to a wide range of topics in both quantum many body physics and quantum information. Often it can be the case that when a family of quantum marginals are compatible with a global quantum state, that global state is unique. This thesis explores the role of uniqueness in the quantum marginal problem, in particular the distinction between uniqueness among pure states and uniqueness among all states. A particularly important variant of the quantum marginal problem is the symmetric extendibility problem. This thesis makes headway on characterizing the extremal points of a particular class of symmetric extendibility problems, and demonstrates the importance of understanding the distinction between being uniquely determined among mixed states and being uniquely determined among pure states in making further progress in this direction.

To my wife Radha, for being my greatest inspiration.

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Chapter 0

Preliminaries

> A map is not the territory it represents, but, if correct, it has a similar structure to the territory, which accounts for its usefulness.
>
> Alfred Korzybski *Science and Sanity (1933, p. 58)*

0.1 The Quantum Formalism

I would like to begin by presenting a set of meta-scientific assumptions which I will use to motivate the notion of a quantum state. Science has primarily concerned itself with generating the tools necessary for people to make successful predictions about the world. The most essential of these tools is the physical theory. Implicit in the idea of prediction is a distinction between the past, which is embodied by what is known, and the future, about which we wish to make predictions. Physical theories assign credences to propositions about the future given what is known about the world. These credences are codified in the form of state. A state is a function that maps from the set of possible propositions to a value in the interval $[0, 1]$, corresponding to the probability that the proposition will be found to be true. Physical theories are maps from the space of what can possibly be known onto the space of states. Note that this implies that in every physical theory the state codifies knowledge. This is not to say that the notion of state as it is traditionally used in science does not

bear ontological significance, but rather that the way we access ontology in science is through predictive schemes. It is how the theory renders certain knowledge redundant and relates states together that codifies its ontological content.

The above theory framework remains true for quantum physcs. In the case of quantum physics, propositions admit a codification into projectors acting on a complex Hilbert space, and quantum states are linear functions which can act on those projectors. These are empirically motivated codifications. The reason they work remains compelling and mysterious. Nevertheless we can formalize these points as follows:

A quantum Hilbert space $\mathbb{H}$ is a complex vector space equipped with a complex inner product. Employing Dirac notation, a vector in $\mathbb{H}$ is expressed with a ket $|\cdot\rangle$. Vectors expressed this way are assumed to be normalized unless otherwise stated. The inner product of two vectors v and u is expressed as $\langle v|u\rangle$. A rank 1 projector onto the vector space spanned by $|v\rangle$ is expressed as $|v\rangle\langle v|$.

A quantum state is a function w which maps from the rank 1 projectors, which codify certain atomic propositions, onto a value in the interval $[0, 1]$, corresponding to the probability that those propositions would be found to be true if measured. More sophisticated propositions can be constructed by combing rank 1 projectors into higher rank projectors associated with subspaces of the Hilbert space. If one proposition entails the negation of another proposition, then their projectors must map into orthogonal subspaces of $\mathbb{H}$. This satisfies the general formulation of a physical state.

By the spectral theorem, every operator which acts on a Hilbert space can be decomposed into a sum of rank 1 projectors. As such, the quantum state is not only a function acting on the projectors of a Hilbert space, but, by its linearity, also a function acting on any operator acting on the Hilbert space. The set of linear operators acting on a Hilbert space $\mathbb{H}$ forms an algebra of bounded operators $B(\mathbb{H})$ equipped with an adjoint operation $(\cdot)^\dagger$. These include unitary operators, which are all those operators U which satisfy $UU^\dagger = \mathbb{1}$ as well as hermitian operators which are all those operators A that satisfy $A = A^\dagger$. As such we may define a quantum state more generally as a linear function on $B(\mathbb{H})$. To satisfy the constraint that

the quantum state map propositions to probabilities, it must also be normalized and positive. Given these conditions we can then define a quantum state associated with a given Hilbert space $\mathbb{H}$ as a function w of the form

$$\begin{aligned} &w : B(\mathbb{H}) \to \mathbb{C} \\ &w(a^\dagger a) \geq 0 \; ; \forall a \in B(\mathbb{H}) \\ &w(\mathbb{1}) = 1 \end{aligned}$$

and denote the set of quantum states associated with a given Hilbert space as $Q(\mathbb{H})$.

If one associates numerical values $\{\lambda_i\}$ with families of mutually orthogonal projectors $\{|i\rangle\langle i|\}$, one can construct operators which codify experiments. The experiments these operators encode seek to decide which proposition among the family of propositions encoded by the set of mutually orthogonal projectors is true. The experiment returns a particular value associated with each proposition. It is sufficient to constrain the values that the experiment outputs to be real numbers, so that the operator $O = \sum_i \lambda_i |i\rangle\langle i|$ associated with a given experiment is a hermitian operator. Experiments codified in this way are called observables. The value $w(O) = \sum_i \lambda_i w(|i\rangle\langle i|) = \sum_i \lambda_i p_i$ is the expectation value of the observable O.

An observable of particular importance is the Hamiltonian of a physical system, which is an observable of the energy of a system. The Hamiltonian governs the dynamical evolution of a physical system, which makes its eigenstates of particular physical relevance as stationary states under time evolution. The lowest energy eigenstate of a Hamiltonian is called a ground state and is of particular interest for codifying the low temperature behaviour of quantum systems.

Every function $w : B(\mathbb{H}) \to \mathbb{C}$ admits a representation ρ given by the equality [1]

$$w(a) = \mathrm{Tr}(\rho a), \; \rho \in B(\mathbb{H}).$$

Consequently the operator ρ, which we call the density matrix, and the quantum state w are often thought of as being synonymous. As such I will use them interchangeably. However from a thematic perspective I will tend to use the function w when I am attempting to take an expansive and abstract stance towards the quantum state. And

I will tend to use the density matrix ρ when I am taking a particular and concrete stance towards a quantum state.

The spectrum of a quantum state is the spectrum of its density matrix. When the density matrix is a rank 1 projector we say that the quantum state is pure and may express it as the vector in the Hilbert space associated with the projector, with the implicit assumption that any global phase on the vector has no physical relevance. When the density matrix has rank greater than 1 we say that it is a mixed state. The positivity condition, $w(a^\dagger a) \geq 0 \; ; \forall a \in B(\mathbb{H})$, is equivalent to the condition that the density matrix ρ has non-negative spectrum, which can be denoted $\rho \geq 0$.

Often we will want to compose multiple physical systems together into a larger physical system. This is done in quantum theory by composing two Hilbert spaces $\mathbb{H}_A$ and $\mathbb{H}_B$ into a larger Hilbert space given by their tensor product $\mathbb{H}_A \otimes \mathbb{H}_B$. Given a basis of $\mathbb{H}_A$: $\{|e_i\rangle\}$ and a basis of $\mathbb{H}_B$: $\{|f_i\rangle\}$ the basis of the new Hilbert space $\mathbb{H}_A \otimes \mathbb{H}_B$ is given by pairings of the basis elements of $\mathbb{H}_A$ and $\mathbb{H}_B$: $\{|e_i\rangle \otimes |f_j\rangle\}$, which may be expressed as $\{|e_i f_j\rangle\}$. The tensor product of two vectors $|v\rangle = \sum_i v_i |e_i\rangle$ and $|u\rangle = \sum_j u_j |f_j\rangle$ is given by $|v\rangle \otimes |u\rangle = \sum_{ij} v_i u_j |e_i\rangle \otimes |f_j\rangle$. Finally, the tensor product of two operators $\rho = \sum_{ij} \rho_{ij} |e_i\rangle\langle e_j|$ and $\sigma = \sum_{mn} \sigma_{mn} |f_m\rangle\langle f_n|$ is $\rho \otimes \sigma = \sum_{ijmn} \rho_{ij}\sigma_{mn}(|e_i\rangle \otimes |f_m\rangle)(\langle e_j| \otimes \langle f_n|)$.

We may also wish to decompose physical systems into subsystems. This can be done by employing the partial trace. Given a Hilbert space $\mathbb{H}_A \otimes \mathbb{H}_B$ the partial trace over system B may be given by the map $\mathrm{Tr}_B : B(\mathbb{H}_A \otimes \mathbb{H}_B) \to B(\mathbb{H}_A)$ defined by its action on an operator $\rho = \sum_{ijmn} \rho_{ij;mn}(|e_i\rangle \otimes |f_m\rangle)(\langle e_j| \otimes \langle f_n|)$ as $\mathrm{Tr}_B(\rho) = \sum_{ij} \sum_m \rho_{ij;mm} |e_i\rangle\langle e_j|$. The quantum state associated with $\mathrm{Tr}_B(\rho)$ is called a marginal, and $\mathrm{Tr}_B(\rho)$ is called a reduced density matrix (RDM). The partial trace over system A is defined in a symmetric fashion. Any pure state $\psi \in \mathbb{H}_1 \otimes \mathbb{H}_2$ for which $\rho_1 = \mathrm{Tr}_2(\psi)$ is said to be a purification of ρ_1. Given the important role the partial trace plays in this thesis I think it is important to take a broader perspective on the motivations for and structure of the partial trace. I will devote the next chapter to that end.

0.2 Quantum Information

A density matrix $\rho \in B(\mathbb{H}_A \otimes \mathbb{H}_B)$ is said to be separable if it admits a decomposition into a convex sum of the form $\rho = \sum_i p_i \rho_i^A \otimes \rho_i^B$ with $\sum_i p_i = 1$. In particular, a pure state $|\psi\rangle$ is separable if it can be expressed as $|\psi\rangle = |\psi_A\rangle \otimes |\psi_B\rangle$. If a quantum state is not separable then it is said to be entangled.

Every pure state $|\psi\rangle \in \mathbb{H}_A \otimes \mathbb{H}_B$ admits a decomposition of the form

$$|\psi\rangle = \sum_i^r \sqrt{\lambda_i} |u_i\rangle \otimes |v_i\rangle,$$

with $\langle u_i|u_j\rangle = \delta_{ij}$ and $\langle v_i|v_j\rangle = \delta_{ij}$. A decomposition of this form is called a Schmidt decomposition. The integer r is called the Schmidt rank, and characterizes the entanglement of the pure state $|\psi\rangle$. The Schmidt rank is upper bounded by the smaller of the dimensions of $\mathbb{H}_A$ and $\mathbb{H}_B$. If the Schmidt rank is maximal, and the values λ_i are uniform, then we say that $|\psi\rangle$ is maximally entangled.

It is in general hard to determine if a quantum state is separable. However there does exist a necessary condition for separability. We may define the partial transpose on system B as the following map $(\cdot)^{T_B} : B(\mathbb{H}_A \otimes \mathbb{H}_B) \to B(\mathbb{H}_A \otimes \mathbb{H}_B)$ by its action on a state $\rho = \sum_{ijmn} \rho_{ij;mn} (|e_i\rangle \otimes |f_m\rangle)(\langle e_j| \otimes \langle f_n|)$ as $\rho^{T_B} = \sum_{ijmn} \rho_{ij;nm} (|e_i\rangle \otimes |f_m\rangle)(\langle e_j| \otimes \langle f_n|)$. The partial transpose on system A is defined symmetrically. For a given state $\rho \in B(\mathbb{H}_A \otimes \mathbb{H}_B)$, if ρ^{T_B} has negative eigenvalues, then ρ is not separable. Similarly for ρ^{T_A}. This is the Peres-Horodecki criterion [2], or the positive partial transpose (PPT) criterion. In the cases where both Hilbert spaces $\mathbb{H}_A$ and $\mathbb{H}_B$ are 2 dimensional, or where one is 3 dimensional and the other is 2 dimensional, the PPT criterion is both necessary and sufficient.

The partial transpose is an example of a superoperator, a linear operator acting on $B(\mathbb{H})$. A particularly important family of superoperators are quantum channels. Although formally defined as completely positive trace preserving maps, quantum channels can be more succinctly defined as the set of maps of the form

$$\Lambda(\cdot) = \sum_k A_k \cdot A_k^\dagger, \; A_k \in B(\mathbb{H}),$$

subject to the constraint that $\sum_k A_k^\dagger A_k = \mathbb{1}$.

Chapter 1

Introduction

> Knowledge is not made for understanding; it is made for cutting.
>
> Michel Foucault *Nietzche, Genealogy, History*

One of the most useful conceptual tools in modern science is the division of physical systems into subsystems. Typically these subsystems are strictly smaller than the system of interest, and are often spatially self contained, instead of their identity being distributed throughout the system. Examples of this are abundant, and include water being composed of water molecules, or human bodies being composed of cells. Exceptions to this particular kind of division into subsystems include for example a computer program being a subsystem of a computer, for which there is no clear spatial division, either in scale or location, between the computer and its program. However subsystems of this type are often considered abstract or not as physical as those subsystems with clear spatial and scale boundaries.

One of the reasons why division into spatially isolated subsystems is so compelling in science is because of the locality of physics. All of the known physical forces act in such a way that they can be thought of as being mediated by entities which must travel through space at a bounded rate. Thus causes and effects propagate in such a way that respects scale and location, making it a good choice to decompose a system into spatially isolated subsystems whose causes and effects on one another can be

easily discerned and analysed.

In accordance with this scientific tradition, quantum physics is equipped with a mathematical tool to decompose quantum states into spatially isolated subsystems. This tool is called the partial trace, and serves an indespensible role in understanding quantum systems. However in quantum physics there is a sense in which this tradition of division into spatially isolated subsystems is inadequate for capturing the full structure of ones quantum system. Take the classic example of a pair of maximally entangled spin-$\frac{1}{2}$ particles [3], separated in such a way that they can not be expected to interact with one another within some period of time. If an experimenter concerns themselves solely with the particles as isolated subsystems of the whole, they will fail to recognize the additional structure inherent in their global quantum state. What's more, this additional structure can only be accessed by careful experimental procedure and foresight. Thus the locality of physics not only encourages us to decide to conceptually decompose the world into spatially isolated subsystems, but also, unless particular experimental precautions are put in place, acts as a fundamental epistemological lens on how we perceive the world, insulating us from the non-local structure inherent in quantum states. It is ultimately a desire to understand the nature of this lens which motivates the subject of this thesis.

The reader may recognize the genesis of this notion of an epistemological lens in the allegory of Plato's cave [4]. In Plato's cave, prisoners are kept such that they are only able to perceive shadows cast upon a wall. Being unable to learn about the objects that cast these shadows, the prisoners are left with the belief that the world is composed entirely of shadows. Their modes of gathering and interpreting knowledge, their epistemology, is restricted. Only when one prisoner is freed from their chains do they realize the true nature of the shadows. I would like to suggest that there are very strong parallels to be drawn between this allegory and the role of locality in quantum mechanics, all the way up to the mathematical notion of a shadow or projection.

Formally, the epistemological lens through which the non-local structure of quantum states is filtered is codified in quantum theory by the partial trace. The partial trace is a linear map from the space of possible states of a quantum system to the

space of possible states of a particular subsystem. One of the reasons that this map filters out the non-local structure of the quantum state is that it is not injective, many possible global quantum states can correspond to the same local quantum states. What is more, when one considers a family of subsystems, one can construct a map from the set of possible states of a quantum system to the space of possible states of the family of subsystems. This map is given by the set of partial traces each corresponding to a particular subsystem. This map is not only not injective, it is also not surjective. There exist ostensibly possible states of local subsystems that can not correspond with any global quantum structure of a particular isolated quantum system. This suggests that the lens of locality is not merely epistemologically restrictive, but also ontologically prescriptive. Just the fact that there is a global quantum system, independently of what state it happens to occupy, restricts the nature of the local subsystems, and this restriction is mediated through the partial trace. By way of analogy, not every set of shadows on the wall of Plato's cave can be produced by the objects outside of the cave.

The principle inquiry of this thesis is under what conditions does a particular collection of local subsystems satisfy the ontological prescription of being the image of a larger quantum system under the lens of locality. In other words, when does a collection of quantum states have a valid preimage under the action of the partial trace. The name for the class of questions of this type is the quantum marginal problem.

The quantum marginal problem is a relatively old problem, dating back at least as far as the 1950s in the study of quantum chemistry [5] under the guise of the N-representability problem. It is also known to be a very hard problem, the most general form falling in the QMA-complete computational complexity class [6]. However some significant headway has recently been made. This includes a complete solution to the non-overlapping quantum marginal problem in 2004 [7], and the first instance of a general solution to an overlapping quantum marginal problem in 2014 [8]. Much of this has been spurred by the relevance of the quantum marginal problem to the burgeoning field of quantum information. That is why, despite the significant historical effort put into understanding this problem, and its inherent difficulty, I

expect that a great deal more can be understood. Motivated by this expectation this thesis endeavours to make novel headway by tackling some of the simplest conceivable unanswered questions.

In particular this thesis will focus on two primary questions. One is how to characterize the extremal points of the set of 2-symmetric extendible states. 2-symmetric extendibility is a particular variant of the quantum marginal problem concerned with characterizing the valid marginals of tripartite states $\rho \in B(\mathbb{H}_A \otimes \mathbb{H}_B \otimes \mathbb{H}_{B'})$ which are symmetric under the exchange of the $\mathbb{H}_B$ and $\mathbb{H}_{B'}$ Hilbert spaces. This question has particular relevance for understanding quantum channel capacity. Unfortunately a complete characterization of the extremal points of the set of 2-symmetric extendible states will not be presented, but significant headway will be shown in this direction.

The second question will relate to the uniqueness of a preimage of the partial trace in the quantum marginal problem. Often there is only one global state compatible with a particular set of marginals, and it can be useful to know when this is the case. In particular I will explore the distinction between being uniquely determined among pure states by a set of marginals and being uniquely determined among all states by a set of marginals. This distinction will be shown to strongly inform the previous question about the extremal points of the set of 2-symmetric extendible states.

In chapter 2 I will talk about the physical motivations for the definition of the partial trace, along with a more general definition of the partial trace than presented in the preliminaries. I will also present an interpretation of the partial trace as a projection in a real vector space and introduce the notion of K-locality.

In chapter 3 I will give a broad overview of the quantum marginal problem, including a general definition, some of its applications, and notable instances of solutions to the problem.

In chapter 4 I will review the symmetric extendibility problem, including a variety of its applications in physics and in quantum information in particular. I will then present a construction for a closed form necessary and sufficient condition for pure 2-symmetric extendibility for non-degenerate states, adapted from a similar construction introduced by Darwin W. Smith [9] in their work on the N-representably problem. This will prove an important component of characterizing the extremal points of the

2-symmetric extendible states. I will also show that no simpler condition which might use only the spectra of the marginals can exist.

In chapter 5 I will draw the distinction between a state being uniquely determined among pure states by its marginals and uniquely determined among mixed states by its marginals. I will then present a novel proof that being uniquely determined among pure states does not imply being uniquely determined among all states. I will do this by giving the first known family of states which are uniquely determined among pure states but not among all states by their marginals.

Finally, in chapter 6 I will demonstrate the role uniqueness plays in characterizing the extreme points of the 2-symmetric extendible states. This will include a novel proof demonstrating that for 2-symmetric extendibility, all extremal points of the set of solutions admit extensions which are uniquely determined among pure states, a corollary of which is that a 2-symmetric extendible state is extremal if and only if it is uniquely determined among all states. I will give a characterization of those states with 2-symmetric extensions which are uniquely determined among pure states, and consider the possibility of whether this also characterizes all extremal 2-symmetric extendible states.

Chapter 2

The Partial Trace

> To them, I said, the truth would be literally nothing but the shadows of the images.
>
> Plato *The Republic*

2.1 Introduction

The notion of the partial trace is of central importance to this thesis. As such I feel it necessary to devote some time to understanding the physical motivations for its construction. These physical motivations will lead to a more general definition of the partial trace than presented in the preliminaries, with some interesting consequences. Finally I will present an interpretation of the partial trace as a projection in a real vector space.

2.2 Defining the Partial Trace

An implicit assumption in the tradition of reductionism in science is that the parts of a whole admit a description independently of that whole. This assumption manifests itself in the quantum mechanical formalism as the partial trace. A quantum system can be conceptualized as being composed of parts (or susbsystems), often

formally represented by a tensor decomposition of its Hilbert space. The partial trace can be thought of as a map from a quantum state of such a system, to quantum states associated with its parts. Consider, for example, a collection of qubits. The total Hilbert space of these qubits naturally admits a decomposition into a tensor product of the Hilbert spaces of each qubit in isolation. Given a complete description of the qubits, the partial trace allows us to describe the behaviour of any individual qubit, independently of its brethren. This reduced description, produced by the partial trace, is referred to as a quantum marginal, borrowing language from probability theory. Of course, the essential feature of quantum mechanics is that an ostensibly complete collection of marginals is often insufficient to describe the whole system.

There are three physical principles which motivate any formal definition of the partial trace. The first principle is that given a system with associated quantum state, and some subsystem with associated marginal, both the quantum state and the marginal should agree on predictions made about experiments performed on the subsystem. We can call this principle "consistency". The motivation for this is that the function of the marginal is to describe the behaviour of the subsystem without requiring a complete description of the whole, however in order to be meaningful it should be consistent with the predictions of the whole. The second principle is that changes on the total state made on parts outside of the subsystem (the environment), should not change the marginal associated with that subsystem. We can call this principle "locality". The locality principle is fundamentally a restriction on how a subsystem can be formally defined, and borrows its motivation philosophically from the notion of identity, that to be defined as an individual a subsystem must necessarily be unaffected by actions on those things which it is not identified with [10]. The third principle is that the subsystem must behave like a quantum system. Specifically, the observables of the subsystem must form an algebra. We can call this final principle "physicality".

Given these principles, we can proceed with a mathematical definition of the partial trace. Equiped with a quantum state $w \in Q(\mathbb{H})$ we should like to define a new function which corresponds to the state of a physical subsystem. We can consider a subset $B_S \subset B(\mathbb{H})$. It is here that we must impose that only subsets that are in agree-

ment with the locality condition and the physicality condition correspond to physical subsystems. The subset B_S is in agreement with the physicality condition when it forms a subalgebra of $B(\mathbb{H})$. The locality condition is satisfied when no transformations to the total state acting outside of the subsystem change the subsystem. It is sufficient to consider transformations on the total state as being unitary operators, which have the action

$$w \to w' : w'(a) = \mathrm{Tr}(U\rho U^\dagger a)$$
$$U = e^{ix},\ x \in B(\mathbb{H}),\ x = x^\dagger$$

which can be concisely expressed as $w'(a) = w(e^{-ix}ae^{ix})$. Consider an algebra B and some subset of elements $g \subset B$, we may denote the set of elements generated by g under the operations of the algebra as $\langle g \rangle$. Consider now the generators $g_S : B_S = \langle g_S \rangle$ and $g : B = \langle g \rangle$ such that $g_S \subset g$. A transformation acting outside of a physical subsystem corresponds to the application of a unitary e^{ix} with $x \in \langle g - g_s \rangle$.

So the locality condition requires that B_S satisfy

$$w(e^{-ix}ae^{ix}) = w(a)\ ; \forall w \in Q(\mathbb{H}),\ \forall a \in B_S,\ \forall x \in \langle g - g_S \rangle.$$

Note that if the generators of B_S satisfy the above condition, then all elements of B_S satisfy it. So we can define B_S as

$$g_S = \left\{ a \in g \mid w(e^{-ix}ae^{ix}) = w(a),\ \forall w \in Q(\mathbb{H}),\ \forall x \in \langle g - g_S \rangle \right\}$$
$$B_S = \langle g_S \rangle.$$

Having defined a B_S which satisfies our locality and physicality conditions we can proceed by defining a new function

$$w_S : B_S \to \mathbb{C}$$

with the property that

$$w_S(a) = w(a);\ \forall a \in B_S.$$

This property satisfies the consistency condition. Finally, to retrieve the commonly used construction of the partial trace, we must change the representation of B_S and

w_S to the irreducible representation of B_S [1] The function w_S then defines the image of the action of the partial trace. What follows are some examples of this construction in action.

2.3 Examples

2.3.1 2-qubits

The simplest and most canonical example of the partial trace is on a collection of finite dimensional, distinguishable, quantum systems. For example a pair of qubits, with Hilbert space $H_1 \otimes H_2 = \mathbb{C}^2 \otimes \mathbb{C}^2$. The generators of the 2-qubit algebra are $\mathbb{1}\otimes\mathbb{1}$, $\sigma_x\otimes\mathbb{1}$, $\sigma_z\otimes\mathbb{1}$, $\mathbb{1}\otimes\sigma_x$, $\mathbb{1}\otimes\sigma_z$, where σ_x, σ_z are the standard 1-qubit Pauli operators. An example of a subalgebra is one generated by $\{\mathbb{1}\otimes\mathbb{1}, \sigma_x\otimes\mathbb{1}\}$, however this subalgebra would not satisfy the locality condition, since $e^{-i\sigma_z\otimes\mathbb{1}}\sigma_x \otimes \mathbb{1}e^{i\sigma_z\otimes\mathbb{1}} \neq \sigma_x \otimes \mathbb{1}$. A subalgebra which does satisfy the locality condition is $B_{S_1} = \langle\{\mathbb{1}\otimes\mathbb{1}, \sigma_x\otimes\mathbb{1}, \sigma_z\otimes\mathbb{1}\}\rangle$. This corresponds to a valid subsystem of our 2-qubit system. Expressed in terms of its irreducible representation this algebra takes the form $B_{S_1} = \langle\{\mathbb{1}, \sigma_x, \sigma_z\}\rangle$. We can then define the partial trace over S_2 of w as the linear function $w_{S_1} : B_{S_1} \to \mathbb{C}$ where $w_{S_1}(a) = w(a), \forall a \in B_{S_1}$. The traditional construction of the partial trace employs the density matrix ρ to construct

$$\rho_{S_1} = \sum_i \langle i_2|\rho|i_2\rangle \in B(H_1)\ ; |i_2\rangle \in H_2,$$

which retrieves $w_{S_1}(a) = \mathrm{Tr}(\rho_{S_1} a)$

One might raise an objection that the definition of the partial trace proposed here is unnecessarily obtuse when it retrieves the traditional construction. I ask that the reader consider the next example.

[1] In my opinion, not employing the irreducible representation is superior from a physical perspective, it preserves information about the position of the subsystem with respect to the global system, and it yields a nice physical interpretation about expected measurements outside of the subsystem, namely that there is zero knowledge about them and are states of maximal entropy. For instance, in the 2-qubit example, not employing the irreducible representation of the subalgebra for subsystem 1 yields the density matrix $\rho_{S_1} \otimes \frac{\mathbb{1}}{2}$.

2.3.2 Mode Reduction in Systems of Multiple Fermions

The modes of a fermionic system are a choice of basis elements for a single particle Hilbert space, for example the momenta of an electron in a finite box. There are instances where it can be useful to consider the behaviour of only a subset of the modes of a fermionic system, for example when studying molecular structures [11] or fermions on a lattice. However unlike systems of distinguishable parts, such as in the previous example, the Hilbert spaces of systems of indistinguishable particles do not readily and unambiguously admit a tensor decomposition into subspaces characterized by modes [12] [13]. For those accustomed to the traditional definition of the partial trace, this leaves one wondering how to consider subspaces of this type, or if the notion is ill conceived. However the construction of the partial trace outlined here accommodates this generalization [13].

The Hilbert space of a system of n fermions occupying $m \geq n$ modes is given by the totally antisymmetric subspace of a system of n distinguishable particles

$$\wedge^n \mathbb{H}_1 = Span\left(\frac{1}{\sqrt{n!}}\sum_{\pi\in S_n}(-1)^{parity(\pi)}\bigotimes_i^n |\psi_{\pi_i}\rangle \mid |\psi_j\rangle \in \mathbb{H}_1\right) \subset \bigotimes^n \mathbb{H}_1,$$

each with single particle Hilbert space $\mathbb{H}_1$. Here π is a permutation and element of the the symmetric group S_n and ψ_j is a possible state a single particle could take. We can then define the Fock space of an m mode system as the direct sum of all the possible n fermion systems, ranging from $n = 0$ fermions to $n = m$ fermions:

$$F_m = \left(\bigoplus_{n=0}^m \wedge^n \mathbb{H}_1\right).$$

The Fock space does not canonically decompose into a tensor product of Hilbert spaces associated with individual modes. This motivates the algebra of canonical anticommutation relations (CAR algebra) as a bookkeeping device for handling operations on modes. The algebra is generated by the ladder operators a_i and $a_i^\dagger$, which are associated with the annihilation and creation respectively of a fermion at mode i. The generators satisfy the relations

$$\{a_i, a_j^\dagger\} = \delta_{ij}\mathbb{1},$$

$$\{a_i, a_j\} = \{a_i^\dagger, a_j^\dagger\} = 0,$$

where $\{\cdot,\cdot\}$ is the anti-commutator. We can then consider Fock space to be spanned by states of the form

$$|p_1, p_2, ..., p_m\rangle = \left(\prod_{i=1}^{m} (a_i^\dagger)^{p_i}\right)|0, 0, ..., 0\rangle = \frac{1}{\sqrt{n!}} \sum_{\pi \in S_n} (-1)^{parity(\pi)} \bigotimes_i^n |\phi_{\pi_i}\rangle$$

where $\vec{p} \in \{1, 0\}^m$ is a binary string indicating whether a given mode is occupied or not, and the product $\prod_{i=1}^m (a_i^\dagger)^{p_i}$ must be equipped with an ordering (ie $(a_1^\dagger)^{p_1}(a_2^\dagger)^{p_2} \neq (a_2^\dagger)^{p_2}(a_1^\dagger)^{p_1}$), and $|\phi_j\rangle$ is a single fermion in mode j. Note that these states do not admit a decomposition of the form $|p_1 p_2 ... p_m\rangle = |p_1\rangle \otimes |p_2\rangle ... \otimes |p_m\rangle$. Moreover, there can be no uniquely defined mapping between states of the form $|p_1 p_2 ... p_m\rangle$ and the form $|p_1\rangle \otimes |p_2\rangle ... \otimes |p_m\rangle$ due in part to the freedom in choosing the ordering of the product in our definition.

With the CAR algebra we can define a fermionic quantum state as a function w^f acting on the elements of the CAR algebra, with every observable expressible in terms of the elements of the CAR algebra. The CAR algebra has subalgebras associated with subsets of modes, for example the subalgebra generated by $\{\mathbb{1}, a_1, a_1^\dagger\}$ associated with the first mode. If it is sensible to think about modes as valid physical subsystems, we need this subalgebra to satisfy the locality condition. Defining the generator $g_F : B(F_m) = \langle g_F \rangle$ the locality condition is

$$w^f(e^{ix} a e^{-ix}) = w^f(a) \mid \forall w^f \in Q(F_m),\ \forall a \in B(F_m),\ \forall x \in \langle g_F - \{a_1, a_1^\dagger\}\rangle.$$

However it is straightforward to see that the locality condition does not hold. Consider the majorana unitary $\gamma_2 = a_2 + a_2^\dagger$. Note that $\gamma_2 = \gamma_2^\dagger$ and $\gamma_2^2 = \mathbb{1}$. By the anti-commutation relations we can easily see that

$$w(\gamma_2 a_1 \gamma_2) = w(-a_1 \gamma_2^2) = -w(a_1),$$

which violates the locality condition.

It turns out that in order to think about fermionic modes as valid physical subsystems one needs to consider a different algebra. Consider that Fock space can be

decomposed into a direct sum of even and odd particle number space:

$$F_m = \left(\bigoplus_{n \in Even}^{m} \wedge^n \mathbb{H}_1 \right) \oplus \left(\bigoplus_{n \in Odd}^{m} \wedge^n \mathbb{H}_1 \right) = F_m^E \oplus F_m^O.$$

We may consider the subalgebra $B(F_m)_P$ of $B(F_m)$ which contains all operators of the form $x = x_E \oplus x_O$ with $x_E \in B(F_m^E)$ and $x_O \in B(F_m^O)$. Here the P stands for parity preserving. $B(F_m)_P$ corresponds to the span of the even monomials in $B(F_m)$. The algebra $B(F_m)_P$ may also be decomposed into subalgebras associated with fermionic modes, for example $\{\mathbb{1}, a_1 a_1^\dagger\}$, and these subalgebras do satisfy all of the requirements for valid physical subsystems. Thus, if we define our fermionic quantum states w_f as being functions on $B(F_m)_P$ instead of $B(F_m)$ then mode reduction is well defined. In particular, any density matrix will have the form $\rho = \rho_E \oplus \rho_O$. This corresponds to parity superselection, the physical law that says that states of fermions can not exist in superposition of even and odd numbers. Only once this condition is imposed on our global structure can we speak about mode reduction sensibly [2].

2.3.3 Particle Reduction in Systems of Multiple Fermions

For the sake of future considerations, and as a contrast to mode reduction we can consider particle reduction of a system of multiple fermions. In fact, because the Hilbert space of N fermions $\wedge^N \mathbb{H}_1$ is a subspace of the N fold tensor product of the single particle Hilbert space $\mathbb{H}_1^{\otimes N}$, we are already equipped with the traditional partial trace as outlined for finite dimensional distinguishable quantum systems, so the same traditional partial trace can be applied to a system with a fixed number of fermions for the purposes of particle reduction:

$$B(\wedge^N \mathbb{H}_1) \to B(\wedge^{N-k} \mathbb{H}_1) \subset B(\mathbb{H}_1^{\otimes N}) \to B(\mathbb{H}_1^{\otimes N-k}).$$

However this mapping does not apply to the entire Fock space, and I will not attempt to introduce such a generalization.

[2] This raises the question of which is more fundamental in physics: fermion parity superselection or the existence of local modes.

A further technical point is that the creation and annihilation operators introduced in the previous section do not generate the algebra $B(\wedge^N \mathbb{H}_1)$, since they do not preserve particle number in general. However those operators A in $B(F_m)$ which preserve particle number admit a tensor sum decomposition of the form

$$A = \bigoplus_i [A]_i \mid [A]_i \in B(\wedge^i \mathbb{H}_i).$$

So we can still employ the particle creation and annihilation operator notation, as long as we restrict ourselves to operators which preserve particle number, and we recall that when we say a product of creation and annihilation operators A acts on $\wedge^N \mathbb{H}_1$ we are really referring to $[A]_N$.

This distinction is important in the context of the partial trace. When we map from $B(\wedge^N \mathbb{H}_1) \to B(\wedge^{N-k} \mathbb{H}_1)$ the operators generated by our creation and annihilation operators also change, going from $[A]_N$ to $[A]_{N-k}$, and critically, for normalized marginals, $w_N([A]_N) \neq w_{N-k}([A]_{N-k})$. Consider for example the particle number operator $N_i = a_i^\dagger a_i$ where here the subscript i indexes mode. We can consider the operator $[N_i]_N$ acting on $B(\wedge^N \mathbb{H}_1)$, and the operator $[N_i]_{N-k}$ acting on $B(\wedge^{N-k} \mathbb{H}_1)$. For a system of N particles, $\sum_i [N_i]_N = N\mathbb{1}$ while for a system with $N-k$ particles $\sum_i [N_i]_{N-k} = (N-k)\mathbb{1}$. If we consider the state w_N, and trace out k particles to retrieve w_{N-k} we should expect that $\sum_i w_N([N_i]_N) = N$ and $\sum_i w_{N-k}([N_i]_{N-k}) = N-k$, however this would not be possible if $w_N([N_i]_N) = w_{N-k}([N_i]_{N-k})$. So instead we must require that

$$w_N([N_i]_N) = w_{N-k}\left(\frac{N}{N-k}[N_i]_{N-k}\right).$$

These points are only really essential when we discuss N-representability, but I think they are worth spending time considering, since fermionic operators are often applied in this fashion in the literature without an explicit account of this subtlety.

2.4 The Partial Trace as a Projection

There is a nice picture that goes along with the partial trace. The space of bounded operators over a Hilbert space $B(\mathbb{H})$ is also a Hilbert space, endowed with the inner

product $\langle a, b\rangle = c_1 \operatorname{Tr}(a^\dagger b)$ [14], this space is referred to as Hilbert-Schmidt space to avoid confusion with the Hilbert space of the quantum system. The real number c_1 is a proportionality factor that we can choose. Given that $w(a) = \operatorname{Tr}(\rho a)$ it seems natural to set $c_1 = 1$ so that $w(a) = \langle \rho, a\rangle$. For a Hilbert space of dimension d, the Hilbert-Schmidt space dimension is d^2. The density matrix $\rho \in B(\mathbb{H})$ associated with the quantum state $w(a) = \operatorname{Tr}(\rho a)$ admits an expansion over a basis of Hilbert-Schmidt space

$$\rho = \sum_i \alpha_i \sigma_i \ |\alpha_i \in \mathbb{C}, \sigma_i \in B(\mathbb{H}), \langle \sigma_i, \sigma_j\rangle = c_2 \delta_{ij}, \sigma_0 \propto \mathbb{1},$$

and consequently the quantum state also admits the expansion

$$w = \sum_i \alpha_i w_i \ , w_i(a) = \langle \sigma_i, a\rangle.$$

We will refer to the vector $\vec{\alpha}$, excluding the element α_0 since it is fixed by normalization, as the Bloch vector, and refer to the vector $\vec{\alpha_+} = \alpha_0 \oplus \vec{\alpha}$ as the completed Bloch vector. The real number c_2 is an additional proportionality factor which we shall need to consider shortly.

If the basis is chosen correctly, the Bloch vector can be constrained to the real numbers [15]. An example of such a basis for a quantum system with a d-dimensional Hilbert space would be the generalized Gell-Mann matrices [15]. The most well known example of this construction is the Bloch ball representation of a qubit, where the 2x2 generalized Gell-Mann matrices are the Pauli matrices. Critically it should be noted that, unlike the case of the Bloch ball ($d = 2$), for $d > 2$ the space of Bloch vectors associated with a valid quantum state do not form a ball, but instead form a complex hyper-dimensional convex shape defined by the condition that the quantum state be positive semi-definite. Some literature refers to this shape as the genearlized Bloch sphere (or ball), I think a more appropriate name is the Bloch spectrahedron, because it is a spectrahedron [16], not a ball.[3] We will refer to the Bloch spectrahedron as Ω, given by

[3] Although a spectrahedron is defined in the literature as $\{\vec{\alpha} \ |a_0 + \sum_i \alpha_i a_i \geq 0 \ , a_i \in Sym_n\}$, where here Sym_n refers to the $n \times n$ real symmetric matrices, there exists a linear invertible map from every hermitian matrix $\sigma_i = A + iB$ to a real symmetric matrix $\begin{bmatrix} A & B \\ -B & A \end{bmatrix}$, so the convex structure of the Bloch spectrahedron remains formally a spectrahedron, despite being over the complex numbers.

$$\Omega(\mathbb{H}) = \left\{ \vec{\alpha} \mid \frac{\mathbb{1}}{\mathrm{Tr}(\mathbb{1})} + \sum_i \alpha_i \sigma_i \, , \sigma_i \in B(\mathbb{H}) \, , \mathrm{Tr}(\sigma_i \sigma_j) = c_2 \delta_{ij} \right\}. \tag{2.1}$$

A basis can also be chosen which makes manifest the partial trace. The elements of the subalgebra associated with a subsystem B_S are closed under addition. This implies that they form a subspace of the Hilbert-Schmidt space (note however that not every subspace forms a valid subalgebra). Since the partial trace $w_S(a)$ satisfies $w_S(a) = w(a)$; $\forall a \in B_S$ it follows that the vector $\vec{\alpha}_S$ associated with w_S is a projection of the vector $\vec{\alpha}$ associated with w into this subspace. We can call the projector Π_S, and its action is given by

$$\vec{\alpha} = \vec{\alpha}_S \oplus \vec{\alpha}_{\bar{S}} \mid \sum_i (\alpha_S)_i \sigma_i \in B_S, \; \sum_i (\alpha_{\bar{S}})_i \sigma_i \notin B_S, \tag{2.2}$$

$$\Pi_S \vec{\alpha} = \vec{\alpha}_S. \tag{2.3}$$

To me this is the most natural picture of the partial trace, as literally a shadow of the quantum state living in a larger space (see figure 2.4).

Finally, with regard to the normalization parameter c_2. The generalized Gell-Mann matrices are standardly defined such that $\mathrm{Tr}(\sigma_i \sigma_j) = 2\delta_{ij}$, however I think it is more convenient from a geometric perspective to scale these matrices such that $\mathrm{Tr}(\sigma_i \sigma_j) = 1$. Consider that if a quantum state is pure, then its density matrix ρ satisfies $\mathrm{Tr}(\rho^2) = 1$. This can be converted into a statement about the completed Bloch vector: $|\vec{\alpha}_+| = 1$.

2.5 K-Locality

In many physically relevant cases a quantum system can be completely decomposed into non-overlapping subsystems, which we can call irreducible subsystems. The 2-qubit example is an instance of such a system, with each qubit being an irreducible subsystem. Under such circumstances we can employ the notion of k-locality. A quantum state is said to be k-local if it is a marginal on at most k irreducible subsystems. In the 2-qubit example, w is 2-local, but not 1-local, while w_{S_1} is both

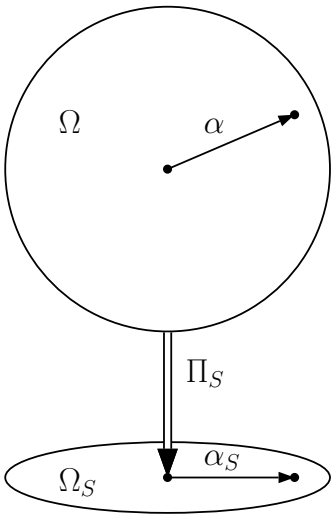


Figure 2.1: An illustration of the action of the partial trace in Hilbert-Schmidt space.

2-local and 1-local. Typically we give a states k-locality in terms of a minimal k. The notion of k-locality extends to observables. An observable O is k-local if its expectation value $w(O)$ depends only on k-local marginals. A generalization can be made by considering subsets K of the power set of irreducible subsystems, which we can refer to as patterns. An example of a pattern for a set of subsystems $\{a, b, c\}$ might be $K = \{\{a, b\}, \{b, c\}\}$. A quantum state is said to be K-local, where K is a pattern, if it is a marginal on a subset of one of the elements of the pattern. Using the previous example a marginal on system a would be K-local, a marginal on system $a \otimes b$ would be K-local, but a marginal on system $a \otimes c$ would not be K-local, as $\{a, c\}$ is neither a subset of $\{a, b\}$ nor $\{b, c\}$. An observable O is K-local if its expectation value $w(O)$ depends only on K-local marginals. With these definitions in mind we can introduce the notion of the K-projection of a Bloch vector ($\vec{\alpha}_K$) as the projection into the union of the subspaces associated with the different subsystems given by the pattern K:

$$\Pi_K := \Pi_{\bigcup S \,|S \in K},$$

$$\vec{\alpha}_K := \Pi_K \vec{\alpha}.$$

What is notable about the K-projection is that it contains only the information necessary and sufficient to specify every K-reduced density matrix. We can note that

an observable O is an hermitian operator in $B(\mathbb{H})$, and as such admits a Bloch vector representation

$$O = \sum_i \theta_i \sigma_i \ , \sigma_0 = \mathbb{1},$$

similar to a reduced density matrix. With this we can say that an observable is K-local if and only if

$$\Pi_K \vec{\theta} = \vec{\theta}.$$

Note that the expectation value of a K-local observable depends only on the information in the K-projection

$$w(O) = \vec{\alpha}.\vec{\theta} = \vec{\alpha}.\Pi_K \vec{\theta} = \vec{\alpha}_K.\vec{\theta},$$

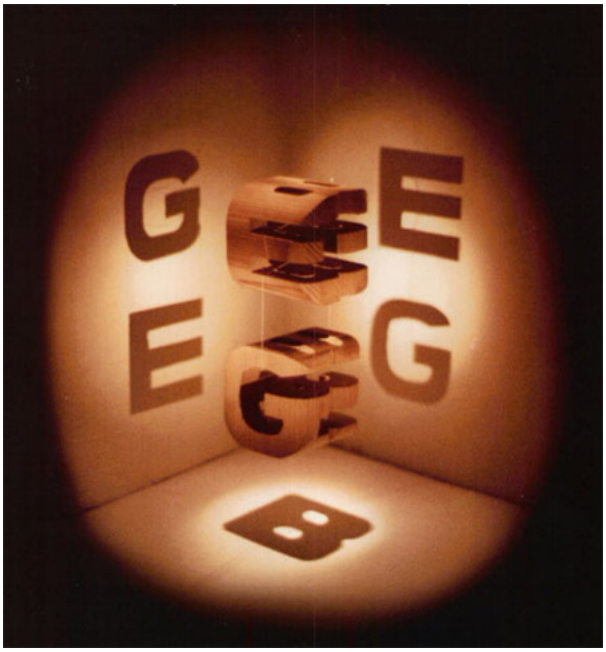
which is as expected.

A final salient definition is the K-shadow of the Bloch spectrahedron

$$\Omega_K = \Pi_K \Omega.$$

Chapter 3

The Quantum Marginal Problem



Douglas R. Hofstadter *Godel Escher Bach*

The image in the epigraph to this chapter is from the cover of the book Godel Escher Bach by Douglas Hofstadter [17][1], which was a very formative book for me. Here it acts as an excellent representation of the quantum marginal problem, although I must credit Matthias Christandl for the idea [18]. Consider the following question:

[1]Reproduced with permission.

for which triplets of letters can such an image be made? That is to say, for a set of three letters, does there exist a block that can cast shadows taking the forms of these letters? [19] For example, I had considered reproducing the image using the letters Q, M and P, for"Quantum Marginal Problem"; however no such block can be constructed! The generalization of this question is: given a collection of projections, does there exist a structure in a higher dimensional space which acts as their projector? As has been discussed in the previous chapter, the marginals of a quantum state can be thought of as projections, or shadows, so there is an equivalent question to be asked about quantum states. Given a collection of quantum marginals, does there exist a quantum state which projects to these marginals via the action of the partial trace? This is the quantum marginal problem. I will now proceed with a more formal definition.

3.1 Definition of the Quantum Marginal Problem

Consider a quantum system, with associated algebra $B(\mathbb{H})$, and consider a set of valid subsystems with associated subalgebras $\{B_i \subset B(\mathbb{H})\}$ and assign to each of these subsystems a quantum state $\{w_i\}$. Does there exist a quantum state

$$w : B(\mathbb{H}) \to \mathbb{C}$$

$$w(a^\dagger a) \geq 0 \; ; \forall a \in B(\mathbb{H})$$

such that

$$w(a) = w_i(a) \; ; \forall a \in B_i, \forall i.$$

If so, $\{w_i\}$ is said to be a *solution* to the quantum marginal problem and w is said to be an *extension*. Some applications of the quantum marginal problem also impose additional constraints on w depending on the physical context, such as symmetry.

The preceding question is an existence question. A natural follow up question arises. If such a quantum state w exists, is it unique? This thesis aims to explore these two questions, existence and uniqueness, as important aspects of the quantum marginal problem.

The quantum marginal problem can be reformulated more naturally in terms of the K-projection. Given a pattern K specifying the collection of subsystems, a spectrahedron Ω and a subset of states of interest $\Gamma \subset \Omega$ (for example symmetric states, or the entire set of states). For which Bloch vectors is it the case that $\vec{\alpha}_K \in \Pi_K\Gamma$, that is to say, which Bloch vectors lie inside the shadow of Γ and therefore correspond to a solution to the quantum marginal problem.

A critical distinction should be made regarding how the subsystems of interest in a quantum marginal problem relate to one another. Quantum marginal problems for which the associated sub-algebras of its subsystems share no common elements, are called *non-overlapping*, because the subsystems do not overlap. Quantum marginal problems for which the associated sub-algebras of its subsystems of interest share common elements are called *overlapping*, because the subsystems overlap.

3.2 Applications for the Quantum Marginal Problem

3.2.1 Symmetric Extendibility

A very special instance of the quantum marginal problem is the symmetric extendibility problem. The symmetric extendibility problem first appeared in quantum chemistry as the N-representability problem, which is of central importance in understanding many-electron systems. It has come to play a central role in quantum information, having relevance in the fields of quantum key distribution, channel capacity and quantum entanglement theory. We shall explore these in detail in the chapter on symmetric extendibility.

3.2.2 Quantum State Tomography

There are many instances where one has an unknown quantum state [20] and one should like to determine what it is. The act of determining an unknown quantum state is called quantum state tomography, and it is of general importance to any science

concerned with quantum mechanical systems. Completely specifying a quantum state with Hilbert space dimension d requires the measurement of the $d^2 - 1$ elements the Bloch vector $\vec{\alpha}$, often referred to as the Stokes parameters in the tomography literature [21]. A major challenge for quantum state tomography is that as quantum systems are combined together, their dimensions are multiplied, so the number of parameters required to specify a quantum state grows exponentially with the size of the whole system. For example the number of real parameters required to specify the quantum state of n qubits is $4^n - 1$, although the number of measurements required can sometimes be less [22]. In some cases it is possible to uniquely determine a quantum state based on its marginals. For such states, the challenge of specifying an exponentially increasing number of parameters through measurement is not an issue. Determining for which states this is the case is an instance of a quantum marginal problem.

3.2.3 Ground States of Local Hamiltonians

Like density matrices, Hamiltonians are operators on $B(\mathbb{H})$, and as such admit a Bloch vector representation, as outlined in the previous chapter,

$$H = \sum_i \theta_i \sigma_i \ , \sigma_0 = \mathbb{1}.$$

The energy of a system with Hamiltonian H in quantum state w is given by $E = w(H)$, which can be re-expressed in terms of Bloch vectors:

$$E = \mathrm{Tr}(\rho H),$$

$$E = \sum_{i,j} \alpha_i \theta_j \, \mathrm{Tr}(\sigma_i \sigma_j),$$

$$E = \sum_i \alpha_i \theta_i.$$

Recalling notation from the previous chapter we can see that

$$E = \vec{\alpha}.\vec{\theta} + \alpha_0 \theta_0.$$

This inner product relation defines a family of affine hyperplanes in the Hilbert Schmidt space, parametrized by energy[23]. Finding the ground state of a Hamiltonian then amounts to finding the $\vec{\alpha}$ vectors which minimize E. We can set θ_0 without loss of physical generality, as it amounts to adding or subtracting constant energy. If we define θ_0 such that the minimal energy is always zero, then we can restrict the set of Hamiltonians to the dual cone of the set of quantum states

$$\mathcal{H} := \{H \mid \langle \rho, H \rangle \geq 0 \ , \forall \rho \in B(\mathbb{H})\}$$

without loss of physical generality.

What's more, the vectors $\vec{\theta}$ define supporting hyperplanes of the Bloch spectrahedron Ω. A face F of a convex set C is a convex subset of C such that $a, b, x \in C$, $x \in F$ and $x \in \{ta + (t-1)b \mid 0 < t < 1\}$ implies $a, b \in F$. That is to say, a subset of C is a face F if any line segment in C whose interior intersects F is also contained fully in F. We can note that any face of F is also a face of C. We can further define an exposed face F_{exp} as any face for which there exists a supporting hyperplane H of C such that $F_{exp} = C \cap H$. From this it should be clear that the ground state space of a Hamiltonian H is just such an exposed face of the Bloch spectrahedron[23].

A salient fact is that all the faces of a spectrahedron are exposed[16], so every face of the Bloch spectrahedron Ω is exposed. However the projections of spectrahedra are not necessarily spectrahedra, and so their faces are not necessarily always exposed. This will be important shortly.

A Hamiltonian is said to be K-local if its expectation value $w(H)$ depends only on K-local marginals. There is a strong relationship between the ground states of K-local Hamiltonians, and pure states which are uniquely determined by their K-local marginals.

It is easy to show that the non-degenerate ground states of K-local Hamiltonians are uniquely determined by their K-local marginals. For a non-degenerate ground state ψ (I will typically use ψ to refer to pure quantum states), if there were another state with the same K-local marginals as ψ it would necessarily have the same energy expectation value of ψ, by the definition of a K-local Hamiltonian. This would mean that ψ was degenerate, a contradiction.

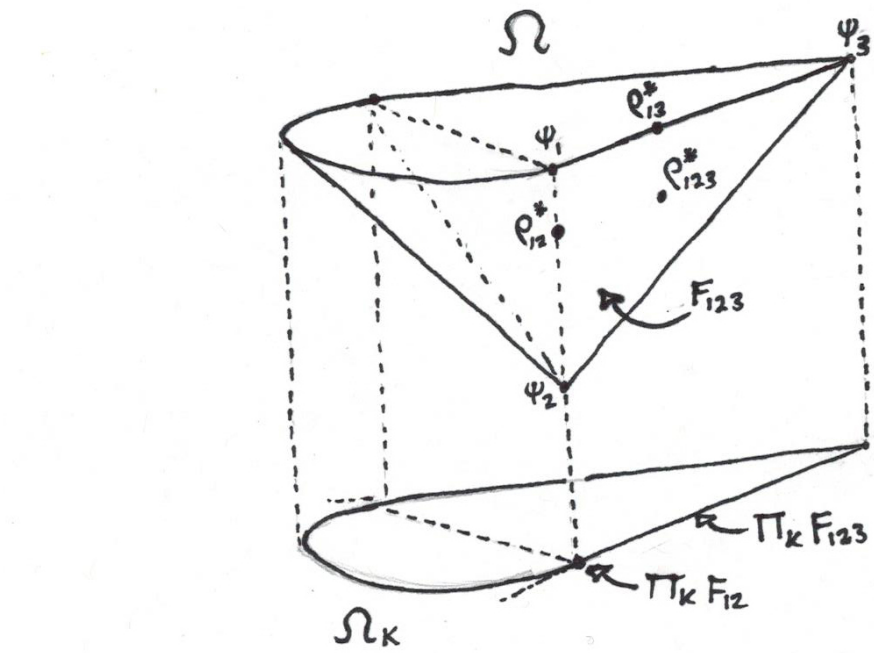


Figure 3.1: An incomplete and distorted representation of some of the features of the Bloch spectrahedron Ω, its K-projection Ω_K, and of K-correlated faces. The face F_{123} generated by the extreme points ψ_1, ψ_2 and ψ_3 is a K-correlated face because the state of maximal entropy on the face ρ^*_{123} is also the state of maximal entropy in the preimage of its projection to the face $\Pi_K F_{123}$ of Ω_K. Note also that $\Pi_K F_{123}$ is also an exposed face, so F_{123} is the ground state space of a K-local Hamiltonian corresponding to the supporting hyperplane intersecting F_{123}. Compare to the face F_{13} formed by the line connecting ψ_1 and ψ_3, it is not a K-correlated face because the state of maximum entropy ρ^*_{13} is not the state of maximal entropy in the preimage of its projection $\Pi_K \rho^*_{13} = \Pi_K \rho^*_{123}$. Finally the face F_{12} is K-correlated but its K-projection is not exposed, so it is not the full ground state space of a K-local Hamiltonian. Note however that the face F_{12} is also not exposed, which would not be the case for a true Bloch spectrahedron.

This is a corollary of a stronger theorem. We can say that a face of Ω is K-correlated if the state of maximum entropy on that face $\rho^* = \sum_i \alpha_i^* \sigma_i$ is also the state of maximal entropy compatible with its K-local marginal (ie its K-projection $\Pi_K \vec{\alpha}^*$). It has been shown that a face is K-correlated if and only if its K-projection is a face of Ω_K. The stronger theorem says that the ground state spaces of K-local Hamiltonians are also K-correlated [23]. Note that a pure state which is uniquely determined by its K-local marginals is also the state of maximal entropy compatible with its K-local marginals, and thus is a 1-dimensional K-correlated space.

One might conjecture that the converse is also true, that any pure state which is uniquely determined by its K-local marginals is the non-degenerate ground state of a K-local Hamiltonian, and more generally that K-correlated faces are always the ground state spaces of K-local Hamiltonians. Unfortunately it is not known if this true. A necessary and sufficient condition for a K-correlated face V to be the full ground state space of a K-local Hamiltonian is that its K-projection $\Pi_K V$ be an *exposed* face of Ω_K[23]. But as mentioned earlier, not all the faces of a projection of a spectrahedron are necessarily exposed.

However it can be shown (see appendix A.1) that every K-correlated space is at least a subspace of the ground state space of a K-local Hamiltonian, even if it is not the full space. Consequently, if a quantum state is uniquely determined by its K-local marginals, then it is certainly a ground state of a K-local Hamiltonian.

3.2.4 The Geometry of Quantum State Space

It is clear from the previous discussion that questions about local Hamiltonians translate naturally into questions about the geometry of the space of quantum states, in particular the geometry of the spectrahedron. Understanding more about the nature of this geometry almost certainly has implications for quantum physics and its sub disciplines such as quantum information and quantum many body physics. This motivates the study of the quantum marginal problem as purely an exercise in understanding the geometry of quantum states, with value in its own right.

3.3 Why is the Quantum Marginal Problem Hard?

It is known that in general the quantum marginal problem is hard. Indeed it is a QMA-complete [24] problem. From the geometric perspective we know that the question amounts to asking whether, given a potential K-projection $\vec{\alpha}_K$, there exists a completion $\vec{\alpha}_{\bar{K}}$ such that the vector $\vec{\alpha} = \vec{\alpha}_K \oplus \vec{\alpha}_{\bar{K}}$ lies within the Bloch spectrahedron. Testing if a given vector lies within the Bloch spectrahedron is not a difficult task and the test can be formulated as follows.

Given a Bloch vector $\vec{\alpha}$, it is inside the Bloch spectrahedron if and only if the trace 1 hermitian matrix $\rho = \sum_i \alpha_i \sigma_i$ satisfies $\rho \geq 0$. The condition $\rho \geq 0$ holds if and only if there exists a purification $\psi \in B(\mathbb{H} \otimes \mathbb{H})$ such $\mathrm{Tr}_2(\psi) = \rho$. The purification, if it exists, can be expressed as $\psi = \sum_{ij} \beta_{ij} \sigma_i \otimes \sigma_j$ where $\beta_{i0} \,\mathrm{Tr}(\sigma_0) = \alpha_i$.

A trace 1 hermitian matrix ψ which is not known to be positive semidefinite is pure if and only if $\psi^2 = \psi$. This condition can be re-expressed in terms of the Bloch vector as

$$\psi^2 = \sum_{ij;mn} \beta_{ij}\beta_{mn}(\sigma_i\sigma_m) \otimes (\sigma_j\sigma_n) = \psi = \sum_{pq} \beta_{pq}\sigma_p \otimes \sigma_q.$$

The product of two generalized Gell-Mann matrices (including the normalization adopted in the previous chapter) is given by

$$\sigma_i\sigma_j = \sum_{k=0} z_{ijk}\sigma_k,$$

with $z_{ijk} = \mathrm{Tr}(\sigma_i\sigma_j\sigma_k) \in \mathbb{C}$, $z_{ijk} = z^*_{jik} = z_{kij}$ and $z_{ij0} = \frac{\delta_{ij}}{\sqrt{d}}$. This gives us a family of multivariate polynomials

$$\sum_{ij;mn} \beta_{ij}\beta_{mn} z_{imp} z_{jnq} - \beta_{pq} = 0$$

which must be satisfied.

A collection of known marginals will fix a subset of α_i given by $\vec{\alpha}_K$ to be constant, leaving all other parameters $\vec{\alpha}_{\bar{K}}$ and $\beta_{ij}, j \neq 0$ as free variables. The existence and uniqueness questions of the quantum marginal problem thus translates into the existence and uniqueness of real valued solutions to the above equation, which is a real algebraic geometry problem. Problems of this form are in general very difficult.

3.4 Notable Instance of Solutions to the Quantum Marginal Problem

The most famous instance of a solution to a non-overlapping quantum marginal problem is a corollary of the Schmidt decomposition. Given a pair of non-overlapping marginals w_A and w_B, does there exist a pure state w_{AB} such that w_A and w_B are its marginals. The necessary and sufficient condition for the existence of such a pure state is that w_A and w_B have identical non-zero spectra [14].

In fact a general solution to non-overlapping quantum marginal problems exists which relies only on the spectra of the marginals. The general solution was demonstrated in 2004 in a seminal paper by Klyachko [7]. In particular, Klyachko poses the following question. Consider a pair of marginals w_A and w_B with fixed spectra λ_A and λ_B, under what conditions are these marginals compatible with a state w_{AB} with a given spectrum λ_{AB}? Klyachko demonstrates that any quantum marginal problem of this form yields necessary and sufficient conditions in the form of linear inequalities of the spectra λ_A, λ_B and λ_{AB}. What's more, every non-overlapping quantum marginal problem can be reduced to a collection of problems of this type by a sequence of bi-partitions. Unfortunately the number of linear inequalities increases dramatically with the system dimension.

Despite being equipped with a complete solution to the non-overlapping quantum marginal problem, the overlapping quantum marginal problem remains extremely difficult. At the moment only one known family of solutions exists for the overlapping quantum marginal problem. This is Chen et. al.'s 2014 result for 2 qubit symmetric extendibility[8]. Before presenting that result, I should like to introduce symmetric extendibility. We will return to this result in section 4.4.5.

Chapter 4

Symmetric Extendibility

> [I]t is never true that two substances are entirely alike, differing only in being two rather than one.
>
> Gottfried Wilhelm Leibniz *Discourse on Metaphysics, 1686*

4.1 Introduction

The problem of symmetric extendibility was first motivated by the study of many electron systems in quantum chemistry [5] [9] more than half a century ago. The Hamiltonians of many physically relevant systems are composed of one and two body interactions. Thus in order to evaluate the energy of such systems, it is sufficient to only posses knowledge of the two body correlations, i.e. the reduced density matrices operating on the Hilbert spaces corresponding to two particles. If the particles in ones system are identical, as is the case with electrons, then every two particle reduced density matrix must be identical. This motivates the question: Which two particle density matrices are compatible with a system of N identical particles? In the context of electrons this is called the N-representability problem. Since its conception N-representability has remained an important and active field of research, and has been generalized beyond fermionic systems under the name symmetric extendibility. Symmetric extendibility has played a central role in a number of important develop-

ments in quantum information theory and many body physics. In this chapter we will explore the symmetric extendibility problem. I will define the problem, give a review of some of its applications and some known results, and then conclude with a discussion of a necessary and sufficient condition for pure symmetric extendibility, adapted from techniques from quantum chemistry for the context of quantum information.

4.2 Definitions

We can define the symmetric extension problem as a constrained version of the quantum marginal problem. Consider a quantum system, with associated algebra $B(\mathbb{H})$, and consider a set of N valid subsystems with associated subalgebras $\{B_i \subset B(\mathbb{H})\}$ such that $\bigcup_i B_i = B(\mathbb{H})$ and that $B_i \approx B_j$, where here equivalence means the subalgebras have the same structure, but are associated with physically distinct subsystems. If one assigns to each subsystem the same quantum state, that is to say, if each subsystem is associated with a marginal w_i such that $w_i \approx w_j$ for all i, j, then does there exist a quantum state

$$w : B(\mathbb{H}) \to \mathbb{C}$$

$$w(a^\dagger a) \geq 0 \; ; \forall a \in B(\mathbb{H})$$

such that

$$w(a) = w_i(a) \; ; \forall a \in B_i, \forall i.$$

If the answer to the above question is in the affirmative, then we can say that the state w is a *N-symmetric extension* of w_i, and that w_i is *N-symmetric extendible*. Furthermore, if there exists a w which is pure, then it is said to be a *pure N-symmetric extension*, and that w_i is *pure N-symmetric extendible*.

The critical constraint is that every marginal be identical. We shall see that this is equivalent to saying that there exists a global state which is symmetric under the exchange of any of the salient subsystems. We can define the *swap operator* $S_{ij} \in B(\mathbb{H})$ with respect to a set of equivalent subsystems $\{B_i \subset B(\mathbb{H})\}$ with $B_i \approx B_j$

as the hermitian special ($det(S_{ij}) = 1$) unitary operator which has the adjoint action

$$Ad_{S_{ij}}(B_i) = S_{ij}B_iS_{ij} = B_j \mid \forall i, j.$$

We can say that a quantum state w is *symmetric* under the exchange of its subsystems if

$$w \circ Ad_{S_{ij}} = w \mid \forall i, j.$$

It follows that the density matrix ρ associated with w satisfies $S_{ij}\rho S_{ij} = \rho$.

If w is symmetric under the exchange of its subsystems then it is easy to show that the marginals of those subsystems are identical. To see this note that the marginal associated with subsystem i is given by $w_i(a_i) = w(a_i) \mid a_i \in B_i$. If w is symmetric under the exchange of its subsystems then

$$w_i(a_i) = w(S_{ij}a_iS_{ij}) = w(a_j) = w_j(a_j) \text{ where } a_i \in B_i, a_j \in B_j, a_i \approx a_j.$$

The converse is more subtle. If all the marginals are identical, it may be the case that there exist states compatible with those marginals which are not symmetric. However it is always guaranteed that if compatible states exist, there must always be a symmetric state compatible with those marginals [25]. To see this consider a state w which is compatible with the identical marginals $\{w_i\}$ and is not necessarily symmetric. A symmetric state

$$w_{sym} \propto w + \sum_{i,j \geq i} w \circ Ad_{S_{ij}}$$

can always be constructed which is also compatible with the marginals.

We can introduce additional structure onto the subsystems B_i such that they can be further decomposed into M sub-subsystems. Then, expanding on the naming convention, we would say that a state w_i is $\vec{N}$*-symmetric extendible*, where $\vec{N}$, a vector of M integers, indicates the number of copies of each sub-subsystem in $B(\mathbb{H})$. Consider for example the Hilbert space $\mathbb{H}_A \otimes \mathbb{H}_{B_1} \otimes \mathbb{H}_{B_2}$, with $\mathbb{H}_{B_1} \approx \mathbb{H}_{B_2}$. We might consider the marginals $w_{A,B_1} \approx w_{A,B_2}$. If the marginals are compatible and an extension exists, we might say that $w_{A,B}$ admits a 2-symmetric extension, or, if we wish to account for the sub-subsystems A and B we may say that $w_{A,B}$ admits

a $(1,2)$-symmetric extension. Such a situation is illustrated in figure 4.2. The value N will always be the product of the integers in $\vec{N}$. For example, in a system with structure $A_1A_2B_1B_2B_3C_1C_2$ we could say the state $w_{A,B,C}$ has a $(2,3,2)$-symmetric extension, or less precisely a 12-symmetric extension, as there are 12 possible ways to select an A, B and C sub-subsystem. In general, the structure of the global system need not be specified in the statement of the problem. It is sufficient to consider just the marginal w_i and ask what kind of extensions it admits.

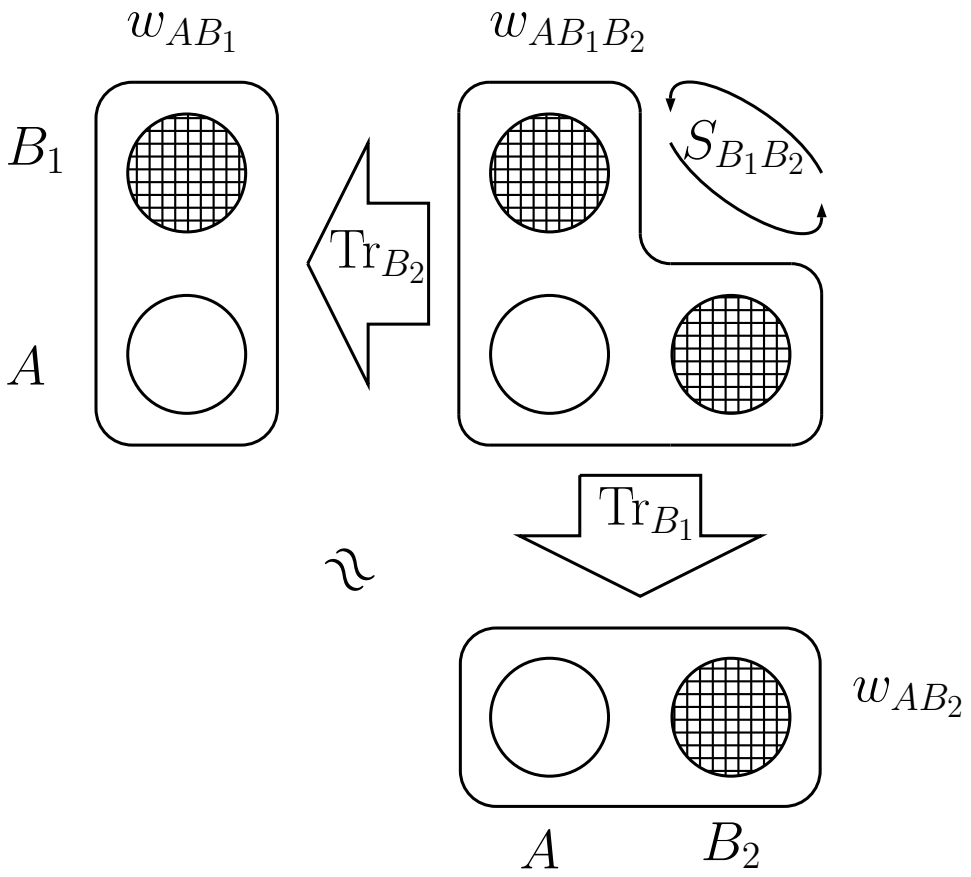


Figure 4.1: An illustration of $\{1,2\}$-symmetric extendibility of a state w_{AB_1}

Finally, we may add a further constraint on the problem in order to make a distinction between bosonic and fermionic symmetries. Noting that $Ad_{S_{iJ}}$ is an involution it follows that $[S_{i,j}^2, x] = 0$ for all elements $x \in B(\mathbb{H})$ and so $S_{i,j}^2 = \mathbb{1}$. This

implies that the spectrum of S_{ij} is $\{1, -1\}$. This implies that $\mathbb{H} = \mathbb{H}_{ij}^{+} \oplus \mathbb{H}_{ij}^{-}$, with $S_{ij}|\psi\rangle = \pm|\psi\rangle,\ \forall|\psi\rangle \in \mathbb{H}_{ij}^{\pm}$. We can define the totally symmetric Hilbert space $\mathbb{H}^{+}$ as the intersection of the positive eigenspaces of each swap operator, $\bigcap_{i,j} \mathbb{H}_{ij}^{+}$, and the totally anti-symmetric Hilbert space $\mathbb{H}^{-}$ as the intersection of the negative eigenspaces of each swap operator $\bigcap_{i,j} \mathbb{H}_{ij}^{-}$. We can then say that a state w is *completely symmetric*, or *bosonic*, if $w(S_{i,j}x) = w(xS_{i,j}) = w(x)\ \forall x \in B(\mathbb{H})$, that is to say, that its density matrix only has support on $\mathbb{H}^{+}$. Similarly, we say that a state w is *completely antisymmetric*, or *fermionic*, if $w(S_{i,j}x) = w(xS_{i,j}) = -w(x)\ \forall x \in B(\mathbb{H})$, equivalently that its density matrix only has support on $\mathbb{H}^{-}$. We can then say that a marginal w_i has a bosonic/fermionic N-symmetric extension if there exists an N-symmetric extension w that is bosonic/fermionic.

4.3 Basic Properties

To establish some intuition about the structure of the symmetric extendibility problem, in particular with regard to (N_a, N_b)-symmetric extension, we should first review some basic facts.

The most important feature of the symmetric extendibility problem is that the set of symmetric extendible states forms a closed convex set. To see this, note that the convex combination of symmetric states is also symmetric and the partial trace is linear. So the convex combination of N-symmetric extendible states is also N-symmetric extendible.

The extremal points of the set of N-symmetric extendible states are pure N-symmetric extendible. Consider that a symmetric state admits a decomposition into a convex combination of pure symmetric states. By the linearity of the partial trace, a symmetric extendible state must admit a similar decomposition into a convex combination of pure symmetric extendible states. However not all pure N-symmetric extendible states are extremal points. Consider that a state ρ may admit a pure N-symmetric extension and also a mixed N-symmetric extension with a decomposition into pure N-symmetric states that are not pure N-symmetric extensions of ρ, in which case ρ is expressible as a convex combination of N-symmetric extendible states

not identical with itself, and consequently is not an extremal point. We shall see in chapter 6 how uniqueness questions in the quantum marginal problem inform when this is the case.

The set of $(1,2)$-symmetric extendible states are closed under local operations and one-way classical communication on systems A and B [26]. This has important consequences for quantum communication.

If a state w_{AB} has a pure $(1,2)$-symmetric extension then it has the same spectrum as its B marginal. Consider a pure symmetric state

$$|\psi\rangle_{ABB'} \in \mathbb{H}_A \otimes \mathbb{H}_B \otimes \mathbb{H}_{B'}.$$

This state admits a Schmidt decomposition

$$|\psi\rangle_{ABB'} = \sum_i \sqrt{\lambda_i}|AB_i\rangle|B_i\rangle,$$

with reduced density matrices

$$\rho_{AB} = \sum_i \lambda_i |AB_i\rangle\langle AB_i|,$$

$$\rho_{B'} = \sum_i \lambda_i |B_i\rangle\langle B_i|.$$

However due to the symmetry of the state $|\psi\rangle$ it must be the case that

$$\mathrm{Tr}_A(\rho_{AB}) = \rho_B = \rho_{B'}.$$

Thus ρ_B and ρ_{AB} share the same spectrum.

In fact, in the case of two qubits, this is a necessary and sufficient condition for pure 2-symmetric extendibility [25]. A natural question to ask is whether this extends to higher dimensions. The following two counterexamples [27] [1], demonstrate that this is not the case:

$$|\psi_{322}\rangle = \frac{1}{\sqrt{6}}|001\rangle + \frac{1}{\sqrt{6}}|110\rangle + \sqrt{\frac{2}{3}}|211\rangle \tag{4.1}$$

$$|\psi_{233}\rangle = \sqrt{\frac{s}{2}}(|121\rangle + |002\rangle) + \sqrt{\frac{1-s}{2}}(|020\rangle + |112\rangle) \tag{4.2}$$

$$s \neq 1/2.$$

[1] Myhr, unpublished correspondence

These states live in a $3 \times 2 \times 2$ and $2 \times 3 \times 3$ dimensional Hilbert space respectively. Neither of the reduced density matrices of these states have a symmetric extension, nevertheless they satisfy the spectrum condition.

A question remains however whether some more sophisticated condition could be constructed which uses solely the spectra. I will show that this is not possible for any dimension greater than 2×2.

4.4 Applications

4.4.1 N-representability

As mentioned earlier, the symmetric extension problem was first motivated by the N-representability problem [28]. Consider a system of N fermions which are governed by a 2-local Hamiltonian H, that is to say that there are interactions between no more than 2 particles. We should like to know the ground state energy

$$\min_{w} w(H) = E_0.$$

Where here w must be a pure fermionic state. We can reformulate this in terms of the Bloch vector representation

$$\min_{\vec{\alpha} \in Ext(\Omega_F^N)} (\vec{\alpha}.\vec{\theta} + \alpha_0\theta_0) = E_0.$$

Where here $Ext(\Omega_F^N)$ is the set of extreme points of the spectrahedron corresponding to the system of N fermions. For the sake of notational convenience we are free to choose $\theta_0 = 0$. Since H is 2-local its ground energy is determined by the 2 particle marginals and we need only consider searching in the 2-projection of $Ext(\Omega_F^N)$ so that

$$\min_{\vec{\alpha_2} \in \Pi_2 Ext(\Omega_F^N)} \vec{\alpha_2}.\vec{\theta} = E_0,$$

recalling that Π_2 is the 2-projection.

Finally, because fermionic states are totally antisymmetric each 2-particle marginal is the same as every other 2-particle marginal. This implies a high degree of redundant information in $\vec{\alpha}_2$. To see this we can decompose the Bloch vector of the marginal

associated with particles i and j into single particle Bloch vectors $\vec{\alpha}_{\{i\}}$, $\vec{\alpha}_{\{j\}}$ and the purely two particle correlation $\vec{\alpha}_{\{i,j\}/(\{i\},\{j\})}$ giving us that

$$\vec{\alpha}_{\{i,j\}} = \vec{\alpha}_{\{i\}} \oplus \vec{\alpha}_{\{j\}} \oplus \vec{\alpha}_{\{i,j\}/(\{i\},\{j\})}.$$

Noting that, due to the particle symmetry, $\vec{\alpha}_{\{i\}} = \vec{\alpha}_{\{j\}} = \vec{\alpha}_{\{1\}}$ and $\vec{\alpha}_{\{i,j\}/(\{i\},\{j\})} = \vec{\alpha}_{\{1,2\}/(\{1\},\{2\})}$ we see that the 2-projection decomposes into

$$\vec{\alpha}_2 = \left(\bigoplus_i^N \vec{\alpha}_{\{i\}} \right) \oplus \left(\bigoplus_{i,j>i}^N \vec{\alpha}_{\{i,j\}/(\{i\},\{j\})} \right),$$

which can be expressed more concisely as

$$\vec{\alpha}_2 = (\vec{\alpha}_{\{1\}})^{\oplus N} \oplus (\vec{\alpha}_{\{1,2\}/(\{1\},\{2\})})^{\oplus N(N-1)/2}.$$

The Bloch vector of the Hamiltonian maintains a similar decomposition due to its fermionic symmetry, taking the form

$$\vec{\theta} = (\vec{\theta}_{\{1\}})^{\oplus N} \oplus (\vec{\theta}_{\{1,2\}/(\{1\},\{2\})})^{\oplus N(N-1)/2}.$$

Thus the energy takes the form

$$\min_{\vec{\alpha}_{\{1,2\}} \in \Pi_{\{1,2\}} Ext(\Omega_F^N)} \left(N \left(\vec{\alpha}_{\{1\}} \cdot \vec{\theta}_{\{1\}} \right) + \frac{N(N-1)}{2} \left(\vec{\alpha}_{\frac{\{1,2\}}{(\{1\},\{2\})}} \cdot \vec{\theta}_{\frac{\{1,2\}}{(\{1\},\{2\})}} \right) \right) = E_0,$$

which may be be expressed more familiarly as

$$\min_{w_2 \in \mathrm{PFSE}} N w_1(H_1) + \frac{N(N-1)}{2} w_2(H_2) = E_0,$$

where w_2, w_1 are two and one particle marginals, PFSE are the set of 2-particle marginals with a pure fermionic N-symmetric extension and H_1, H_2 are one and two particle interaction terms.

Although this space is significantly smaller, there remains the problem of deciding if a marginal admits a pure fermionic N-symmetric extension. This decision problem is the N-representability problem.

4.4.2 Generalized Pauli Constraints

Although the N-representability problem is in general hard, necessary conditions for a marginal to admit a pure fermionic N-symmetric extension can be considered, for example, conditions on the single particle marginals. Thanks to Klyachko's work on the pure univariant quantum marginal problem, necessary conditions of this type can be constructed, and they will all take the form of spectral conditions. The spectra $\vec{\lambda}$ of single particle marginals of fermionic systems are typically referred to as natural occupation numbers and the eigenvectors as natural orbitals in the quantum chemistry literature. Note that the natural orbitals are not always the same as the canonical choice of modes of a single fermion, especially for interacting fermionic systems, however a local unitary transformation can always generate a new set of creation and annihilation operators associated with the natural orbitals. Most quantum chemistry literature treats the single particle marginal as non-normalized, so that $\sum_i \lambda_i = N$, however here we will stick to normalized systems so that $\sum_i \lambda_i = 1$.

The first spectral condition of the N-representability problem predates Klyachko by nearly 80 years. I am referring of course to the Pauli exclusion principle, the normalized version of which is

$$0 \leq \lambda_i \leq \frac{1}{N}, \forall i.$$

The original formulation of the principle was not couched in the terms used here, but it is ultimately a spectral constraint in the quantum marginal problem. Its proof follows directly from the structure of the CAR algebra and some of the subtleties discussed in chapter 2.

Consider an N fermion state w_N with single particle reduced density matrix w_1. The number operator $N_i = a_i^\dagger a_i$ is idempotent since

$$N_i^2 = a_i^\dagger a_i a_i^\dagger a_i$$

$$N_i^2 = a_i^\dagger (-a_i^\dagger + \mathbb{1}) a_i$$

$$N_i^2 = a_i^\dagger a_i = N_i.$$

This implies that it has eigenvalues 1 or 0, and so its expectation value is similarly bounded by

$$0 \leq w_N(N_i) \leq 1.$$

Recalling that $w_N(N_i) = N w_1(N_i)$ we can see that

$$0 \leq w_1(N_i) \leq \frac{1}{N}.$$

And finally, the number operator acting on the 1 particle space takes the form of a rank 1 projector, and so returns the diagonal elements of ρ_1. Thus the inequality holds for the eigenvalues, and we retrieve our spectral inequality.

In fact, the Pauli exclusion principle is not only a necessary condition for pure fermionic N-symmetric extendibility, but also a necessary and sufficient condition for mixed fermionic N-symmetric extendibility of the single particle marginals [29].

The significance of the exclusion principle can not be overstated, having fundamental bearing on the general structure of matter. This warrants exploring other single particle spectral constraints in the N-representability problem. These additional constraints are referred to as generalized Pauli constraints.

The next set of constraints were proposed by Borland and Dennis in the 70s [30] although a proof was only supplied much later by Ruskai in 2007 [31]. This set of single particle spectral constraints is for pure fermionic 3-symmetric extendibility with 6 modes and are

$$\lambda_1 + \lambda_6 = \lambda_2 + \lambda_5 = \lambda_3 + \lambda_4 = \frac{1}{6},$$

$$\lambda_4 \leq \lambda_5 + \lambda_6,$$

$$\lambda_i \leq \lambda_{i+1}.$$

Finally, Klyachko provided a procedure for generating a complete set of single particle spectral constraints for there to be a pure N-fermionic symmetric extension, given any number of particles and modes.

With the full set of generalized Pauli constraints at hand, there is an ongoing research programme to find physical models which demonstrate such constraints [29].

4.4.3 The Quantum De-Finetti Theorem and an Infinite Family of Separability Conditions

The quantum De-Finetti theorem is a quantum analogue of a theorem in classical Bayesian probability theory about how to account for the notion of an unknown probability. If the assignment of a probability is conceived of as a reflection of ones state of knowledge, then how does one conceptualize the notion of an unknown probability? This same difficulty arises in quantum foundations when we consider the notion of an unknown quantum state [20]. The solution is to formulate any statements about unknown probabilities or quantum states into statements about repeated symmetric preparation procedures, the probabilistic outcomes of which have certain properties due to the symmetry of the preparation. In fact, the quantum De-Finetti theorem is a solution to a specific case of the symmetric extendibility problem, and closely connects the symmetric extendibility problem to characterizing separability in quantum states.

Consider a preparation procedure that can produce any number of identical quantum state preparations. We may say that the total output of N uses of the preparation procedure gives us the quantum state w_N. Since the preparation procedure is symmetric we may say any single use of the preparation procedure gives the same marginal w_1. We may say then that w_1 admits an N-symmetric extension w_N. What's more, we have assumed that the preparation procedure can produce any number of identical quantum state preparations, so w_1 admits an N-symmetric extension for all N. The simplest form of the quantum De-Finetti theorem tells us the following. For symmetric states w_k with density matrices $\rho_k \in B(\mathbb{H}_1^{\otimes k})$, if w_k admits for all N a symmetric extension w_N with density matrix $\rho_N \in B(\mathbb{H}_1^{\otimes N})$ such that

$$\rho_k = \mathrm{Tr}_{N-k}(\rho_N).$$

Then ρ_k admits the separable decomposition

$$\rho_k = \sum_i P_i \rho_i^{\otimes N} \mid \rho_i \in B(\mathbb{H}_1),$$

and in particular

$$\rho_1 = \mathrm{Tr}_{k-1}(\rho_k) = \sum_i P_i \rho_i.$$

This classical probability distribution over ρ_i operationalizes the notion of an unknown quantum state as a marginal of a potentially infinite sequence of identical preparations.

From this we can see that if a multiparty system admits an N-symmetric extension for any N, then that system is separable over those parties. However more can be said by considering a more sophisticated form of the quantum De-Finetti theorem [32] [33].

Let $\rho_N \in B(\mathbb{H}_1^{\otimes N})$ be the density matrix of a symmetric state w_N with $dim(\mathbb{H}_1) = d$. Let $\rho_k \in B(\mathbb{H}_1^{\otimes k})$ be the reduced density matrix associated with the k-particle marginal w_k of w_N. Then there exists a separable state

$$\Gamma_k = \sum_i P_i \gamma_i^{\otimes k} \mid \gamma_i \in B(\mathbb{H}_1)$$

such that

$$||\rho_k - \Gamma_k||_1 < \frac{4d^2k}{N},$$

where $||x||_1 = \mathrm{Tr}(\sqrt{x^\dagger x})$.

It is clear that if a state admits an N-symmetric extension then it also admits an $N-1$-symmetric extension, and so if we consider all possible k party states, and we classify them in terms of the degree of symmetric extension they admit, then these classes are nested within one another, such that the N-symmetric extendible states lie within the $N-1$-symmetric extendible states. From the quantum De-Finetti theorem we can see that these nested classes converge on the set of separable states as N approaches infinity (see figure 4.4.3).

4.4.4 Anti-degradable Channels

The action of a quantum channel $\Lambda : B(\mathbb{H}_A) \to B(\mathbb{H}_A)$ on a density matrix $\rho \in B(\mathbb{H}_A)$ can always be thought of as the evolution of ρ as it interacts with some

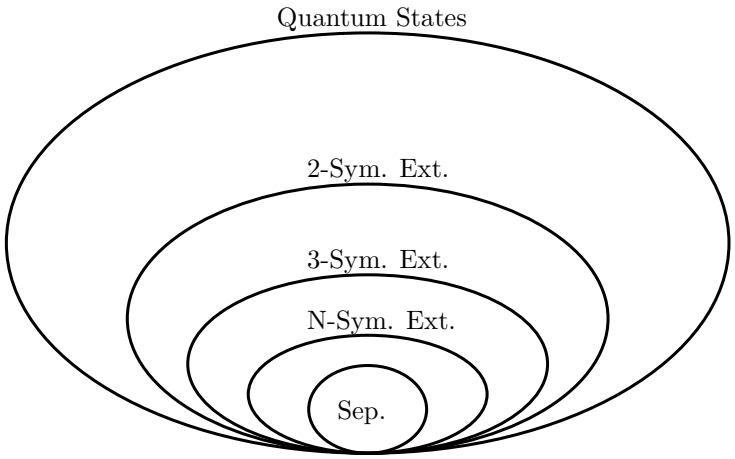


Figure 4.2: Each set of N-symmetric extendible states is nested within the $N-1$-symmetric extendible states. In the limit that N approaches infinity the N-symmetric extendible states coincide precisely with the separable states.

environment. This can be represented by the A marginal of a bipartite unitary $U_{AE} \in B(\mathbb{H}_A \otimes \mathbb{H}_E)$ acting on ρ composed with a pure environment density matrix

$$\Lambda(\rho) = \mathrm{Tr}_E(U_{AE}(\rho \otimes |0\rangle\langle 0|_E)U_{AE}^\dagger).$$

If instead the E marginal is considered, we retrieve the action of the complementary channel

$$\Lambda_c(\rho) = \mathrm{Tr}_A(U_{AE}(\rho \otimes |0\rangle\langle 0|_E)U_{AE}^\dagger).$$

A channel is always a complementary channel of its complementary channel.

A channel Λ is said to be degradable if there exists a channel $\mathbb{D}$ such that $\Lambda_c = \mathbb{D} \circ \Lambda$. Alternatively Λ is said to be anti-degradable if there exists a degrading channel $\mathbb{D}$ such that $\Lambda = \mathbb{D} \circ \Lambda_c$. The complementary channel of a degradable channel is anti-degradable, and vice versa. There is a strong sense in which channels funnel quantum information out of system A and into system E. Degradable channels are those channels which preserve enough quantum information in system A to reconstruct system E, and anti-degradable channels are the converse. We should note here that complementary channels are not strictly unique, however there exists a partial isometry between any two complementary channels such that for any two channels $\Lambda_{c_1}, \Lambda_{c_2}$ which are complementary to Λ, if one can be degraded to Λ, then so can the

other [34].

A channel acting on $B(\mathbb{C}^d)$ can be expressed uniquely as a bipartite quantum state by considering its action on one half of a generalized Bell state $|\phi^+\rangle = \frac{1}{\sqrt{d}} \sum_i^d |i\rangle|i\rangle \in B(\mathbb{C}^d \otimes \mathbb{C}^d)$:

$$\rho_\Lambda = \mathbb{1} \otimes \Lambda(|\phi^+\rangle\langle\phi^+|).$$

The quantum state ρ_Λ is referred to as the Choi matrix representation of the channel (with some definitions varying normalization).

There is a tight relationship between the anti-degradable channels and symmetric extendible states. Indeed a channel is anti-degradable if and only if its Choi matrix is (1,2)-symmetric extendible [25]. The proof is as follows. Consider the tripartite state associated with a channel Λ acting on a system of interest A, with a reference system R which the system of interest is entangled with, and an environment E, given by

$$\rho_{RAE} = (\mathbb{1}_R \otimes U_{AE})(|\phi^+\rangle\langle\phi^+| \otimes |0\rangle\langle 0|_E)(\mathbb{1}_R \otimes U_{AE})^\dagger.$$

We see that $\rho_\Lambda = \mathrm{Tr}_E(\rho_{RAE})$ and $\rho_{\Lambda_c} = \mathrm{Tr}_A(\rho_{RAE})$. What's more, ρ_{RAE} is a purification of both ρ_Λ and ρ_{Λ_c}. Note that for any purification of ρ_Λ the purifying space can be thought of as an environment E

If the channel Λ is anti-degradable, then there exists a degrading channel $\mathbb{D}$ acting on E such that $\mathbb{D} \circ \Lambda_c = \Lambda$. Applying this channel we produce a new state

$$\rho_{RAA'} = \mathbb{1}_R \otimes \mathbb{1}_A \otimes \mathbb{D}_E(\rho_{RAE})$$

such that

$$\rho_\Lambda = \mathrm{Tr}'_A(\rho_{RAA'}) = \mathrm{Tr}_A(\rho_{RAA'}).$$

We see that ρ_Λ admits a (1,2)-symmetric extension if Λ is anti-degradable.

Suppose now we have a state ρ_{RA} corresponding to the Choi matrix of a channel Λ. Suppose ρ_{RA} admits a (1,2)-symmetric extension $\rho_{RAA'}$ such that $\rho_{RA} = \rho_{RA'}$. We can consider a purification of this extension $\psi_{RAA'P}$ with P the purifying space. We can note that this is also a purification of ρ_{RA}, and so the state $\rho_{RA'P} = \mathrm{Tr}_A(\psi_{RAA'P})$ corresponds to the Choi matrix of a channel Λ_c which is complementary to Λ. There exists a degrading channel $\mathbb{D} = \mathrm{Tr}_P$ acting on the environment $A'P$ such that

$$\mathbb{D}(\rho_{RA'P}) = \mathbb{1} \otimes (\mathbb{D} \circ \Lambda_c)(|\phi^+\rangle\langle\phi^+|) = \rho_{RA'} = \rho_{RA} = \mathbb{1} \otimes \Lambda(|\phi^+\rangle\langle\phi^+|).$$

This implies that Λ is anti-degradable. So Λ is anti-degradable if and only if its Choi matrix ρ_Λ admits a (1,2)-symmetric extension.

Furthermore, since the complementary channel of a degradable channel is always anti-degradable, Λ is degradable if and only if the Choi matrix of its complementary channel ρ_{Λ_c} admits a (1,2)-symmetric extension.

4.4.5 Quantum Key Distribution

A quantum channel can be thought of as a mechanism by which quantum information is shared between two parties separated in space-time, in particular a mechanism by which entanglement is shared. Indeed the Choi matrix of a channel can be thought of as the quantum state shared between two parties, Alice and Bob, after one half of a maximally entangled state is sent through the channel from Alice to Bob. It is well known that as a corollary of the no-cloning theorem, two parties who share a maximally entangled state are capable of securely transmitting classical information between one another without any eavesdropper being able to intercept that information [35] [36]. What's more, two parties who share a maximally entangled state can faithfully transmit any other quantum information between them. This motivates the notion of a channels quantum capacity $Q(\Lambda)$, which should characterize its capacity to share a maximally entangled state between two parties.

Even if a channel is incapable of faithfully transmitting a maximally entangled state, many uses of a channel allow Alice and Bob to have a collection of shared quantum states from which they may extract some number of maximally entangled states through a process called entanglement distillation. It is important to note that depending on the types of classical communication available to Bob and Alice, different rates of entanglement distillation may be found. In particular, protocols for distilling entanglement which restrict all classical communication to be from Alice to Bob will be strictly weaker than protocols which also allow Bob to communicate with Alice. We shall refer to the former type of protocol as one-way, and the latter as two-way. Historically it has become standard to define quantum capacity $Q(\Lambda)$ as the entanglement distillable from many uses of a channel with one-way classical

communication protocols, in keeping with classical communication theory. This also has a nice operational meaning for characterizing quantum memory. We can conceive of the storing of quantum information in an imperfect quantum memory device as the transmission of quantum information through a noisy quantum channel. However Alice and Bob in this scenario are strictly separated by time, and only one way classical communication is possible through time.

An important quantity for defining the quantum capacity of a channel is the coherent information

$$I(\Lambda) = \max_{\rho \in B(\mathbb{H}_A)} S(\Lambda(\rho)) - S(\Lambda_c(\rho)).$$

One can think of coherent information as a characterization of the entanglement preserved between system A and the reference system R after the action of the channel.

Indeed it is known that if Alice and Bob share an arbitrarily large number of copies of the Choi matrix of the channel, that is to say, Alice sends Bob one half of a maximally entangled state an arbitrarily large number of times times through the channel, then it is possible for them to distill maximally entangled states at a rate of $I(\Lambda)$[37]. The coherent information tells one how many entangled states can be distilled from a number of independent uses of the channel. However the channel uses need not be independent, we may compose channels and entangle their input states. With this in mind we can define the quantum capacity as the achievable rate of distillation for an arbitrarily large composition of channels given by

$$Q(\Lambda) = \lim_{N \to \infty} \frac{I(\Lambda^{\otimes N})}{N}.$$

The degradability or anti-degradability of a channel has consequences for its quantum capacity. There is typically a gap between the actual quantum capacity and the coherent information, such that more capacity can be achieved. However for degradable channels, the quantum capacity is the coherent information

$$Q(\Lambda) = I(\Lambda).$$

The quantum capacity of anti-degradable channels, on the other hand, is known to always be zero. This tells us that anti-degradable channels can not be used to securely

transmit classical information, that they are susceptible to eavesdroppers. To see this we may return to the notion of the Choi matrix ρ_{AB} of a channel representing the shared state of Alice and Bob after Alice transmits one half of a maximally entangled state through the channel to Bob. We can say that if their shared state admits a symmetric extension $\rho_{ABB'}$ then there may exist an eavesdropper represented by the B' space who would possess the same quantum correlation with Alice, the same measurement statistics as Bob and consequently potential access to the same classical information as Bob. This makes (1,2)-symmetric extension of particular interest to the quantum cryptography community[25].

The simplest non-trivial instance of a (1,2)-symmetric extension problem is whether a 2 qubit state ρ_{AB} admits a (1,2)-symmetric extension. In the case where ρ_{AB} is the Choi matrix of a quantum channel Λ, this is equivalent to asking which single qubit channels are anti-degradable. A complete closed form characterization of this problem was first conjecture by Myhr[25], and later proved by Chen et. al. [8]. A 2 qubit state ρ_{AB} admits a (1,2)-symmetric extension if and only if

$$\mathrm{Tr}(\rho_B^2) \geq \mathrm{Tr}(\rho_{AB}^2) - 4\sqrt{\det(\rho_{AB})}.$$

This is the first and only known complete solution to an overlapping quantum marginal problem, and the only known complete characterization of the anti-degradability and consequently degradability of the set of quantum channels of a specific dimension. It bears noting that this condition, although highly non-trivial, can be expressed completely in terms of the spectra of the marginals. We shall see that this is in general not possible for higher dimensional cases.

4.5 Necessary and Sufficient Conditions for Pure 2-Symmetric Extendibility

Given the broad applicability of the symmetric extension problem, even incremental progress may be valuable. With this in mind we turn to one of the simplest questions one might pose. Under what conditions is a bipartite state pure

2-symmetric extendible? This question is important in characterizing the full convex set of 2-symmetric extendible sets, as every extremal point of the set is necessarily pure 2-symmetric extendible.

I shall present here a closed form necessary and sufficient condition for pure 2-symmetric extendibility for non-degenerate states. Importantly, this condition is an extension of a technique developed by Darwin W. Smith in their work on the N-representability problem[9]. In reference [9] Smith gives necessary and sufficient conditions for the pure fermionic 3-representability problem. The construction presented here will take a very similar form, save for the fact that it has been adapted for not only fermionic systems but any symmetric system, and the syntax updated for the modern quantum information community.

I should note that we will be considering pure $(1,2)$-symmetric extendibility as this encompasses all cases of 2-symmetric extendibility.

Theorem 4.5.1. *If ρ_{AB} is a quantum state with eigensystem $\{|g_i\rangle, \lambda_i\}$ and no non-zero degeneracy (i.e. if $\lambda_i = \lambda_j$ then $\lambda_i = 0$), and $\mathrm{Tr}_A(\rho_{AB})$ is a quantum state with eigensystem $\{|f_i\rangle, \gamma_i\}$. Then ρ_{AB} has a pure $(1,2)$-symmetric extension if and only if $\{\lambda_i\} = \{\gamma_i\}$ and there exist a set of phases ϕ_i such that $\langle D_{kj}|D_{jk}\rangle = \pm e^{i(\phi_k - \phi_j)}\langle D_{kj}|D_{kj}\rangle$. Where $|D_{jk}\rangle = \sqrt{\lambda_j}\langle f_k|g_j\rangle \in \mathbb{H}_A$, and $\pm = \begin{cases} +, \textit{Bosonic extension} \\ -, \textit{fermionic extension} \end{cases}$.*

Proof. We begin by proving that if ρ_{AB} has a pure $(1,2)$-symmetric extension, then there exist a set of phases $\{\phi_i\}$ such that $\langle D_{kj}|D_{jk}\rangle = \pm e^{i(\phi_k - \phi_j)}\langle D_{kj}|D_{kj}\rangle$.

Assume ρ_{AB} has a pure $(1,2)$-symmetric extension $|\psi\rangle$ satisfying

$$\begin{aligned} &|\psi\rangle \in \mathbb{H}_A \otimes \mathbb{H}_B \otimes \mathbb{H}_{B'} \\ &S_{BB'}|\psi\rangle = \pm|\psi\rangle \\ &\rho_{AB} = \mathrm{Tr}_{B'}(|\psi\rangle\langle\psi|) = \mathrm{Tr}_B(|\psi\rangle\langle\psi|). \end{aligned} \tag{4.3}$$

Here the plus or minus sign under the exchange operation distinguishes between bosonic and fermionic symmetric extensions respectively.

We can express $|\psi\rangle$ as a Schmidt decomposition between Hilbert spaces $\mathbb{H}_A \otimes \mathbb{H}_B$

and $\mathbb{H}_{B'}$ given by

$$|\psi\rangle = \sum_i \sqrt{\lambda_i}|G_i\rangle_{AB}|F_i\rangle_{B'}. \tag{4.4}$$

Then ρ_{AB} necessarily takes the form

$$\rho_{AB} = \sum_i \lambda_i |G_i\rangle\langle G_i|. \tag{4.5}$$

Noting that $\mathrm{Tr}_{AB'}(|\psi\rangle\langle\psi|) = \mathrm{Tr}_{AB}(|\psi\rangle\langle\psi|)$ it follows that

$$\begin{aligned} \rho_B = \rho_{B'} &= \mathrm{Tr}_{AB}(|\psi\rangle\langle\psi|), \\ \rho_B &= \sum_i \lambda_i |F_i\rangle\langle F_i|. \end{aligned} \tag{4.6}$$

Consider the eigenstates of ρ_{AB} and ρ_B satisfying

$$\begin{aligned} \rho_{AB}|g_i\rangle &= \Lambda_i|g_i\rangle, \\ \rho_B|f_i\rangle &= \Lambda_i|f_i\rangle. \end{aligned} \tag{4.7}$$

Since there is no non-zero degeneracy in the eigenvalues, we can deduce that

$$\begin{aligned} \Lambda_i &= \lambda_i, \\ |g_i\rangle &= e^{i\phi_i^{AB}}|G_i\rangle, \\ |f_i\rangle &= e^{i\phi_i^{B}}|F_i\rangle. \end{aligned} \tag{4.8}$$

By substitution into equation 4.4 we find that

$$\begin{aligned} |\psi\rangle &= \sum_i e^{i\phi_i}\sqrt{\lambda_i}|g_i\rangle_{AB}|f_i\rangle_{B'}, \\ \phi_i &= \phi_i^{AB} + \phi_i^{B}. \end{aligned} \tag{4.9}$$

Recalling that $|\psi\rangle$ is an eigenstate of the exchange operator we find that

$$\sum_i e^{i\phi_i}\sqrt{\lambda_i}S_{BB'}|g_i\rangle_{AB}|f_i\rangle_{B'} = \pm\sum_i e^{i\phi_i}\sqrt{\lambda_i}|g_i\rangle_{AB}|f_i\rangle_{B'}. \tag{4.10}$$

Acting from the left with $\langle f_j|_B \otimes \langle f_k|_{B'}$

$$\begin{aligned} &\sum_i e^{i\phi_i}\sqrt{\lambda_i}\langle f_j|_B\langle f_k|_{B'}S_{BB'}|g_i\rangle_{AB}|f_i\rangle_{B'} \\ &= \pm\sum_i e^{i\phi_i}\sqrt{\lambda_i}\langle f_j|_B\langle f_k|_{B'}|g_i\rangle_{AB}|f_i\rangle_{B'}, \end{aligned} \tag{4.11}$$

$$\begin{aligned} &\sum_i e^{i\phi_i}\sqrt{\lambda_i}\langle f_k|_B\langle f_j|_{B'}|g_i\rangle_{AB}|f_i\rangle_{B'} \\ &= \pm\sum_i e^{i\phi_i}\sqrt{\lambda_i}\langle f_j|_B\langle f_k|_{B'}|g_i\rangle_{AB}|f_i\rangle_{B'}, \end{aligned} \tag{4.12}$$

$$\begin{aligned} &e^{i\phi_j}\sqrt{\lambda_j}\langle f_k|_B|g_j\rangle_{AB} \\ &= \pm e^{i\phi_k}\sqrt{\lambda_k}\langle f_j|_B|g_k\rangle_{AB}. \end{aligned} \tag{4.13}$$

Defining

$$|D_{jk}\rangle = \sqrt{\lambda_j}\langle f_k|g_j\rangle \tag{4.14}$$

we find

$$\langle D_{kj}|D_{jk}\rangle = \pm e^{i(\phi_k-\phi_j)}\langle D_{kj}|D_{kj}\rangle. \tag{4.15}$$

This concludes the proof of the necessary condition. The sufficient condition, that is that if condition 4.15 is true, then ρ_{AB} has a pure symmetric extension, follows constructively.

If there exists a set of ϕ_i such that condition 4.15 is true, then we can always construct a pure symmetric extension of ρ_{AB}, namely the state given in equation 4.9. □

It is worth noting that nowhere has there been made any presumption about the dimensions of the Hilbert spaces involved, so the above theorem holds generally for all dimensions.

Consider now the matrix

$$M_{kj} = \frac{\langle D_{kj}|D_{jk}\rangle}{\langle D_{kj}|D_{kj}\rangle}, \tag{4.16}$$

where we allow undefined elements when $\langle D_{kj}|D_{jk}\rangle = 0$. This is a useful representation, as it allows for quick ruling out of states which obviously do not have a pure $(1,2)$-symmetric extension, such as when defined elements are not roots of unity, or when it is not hermitian. What's more, in the case where M has no undefined elements, it is straightforward to see that in order for ρ_{AB} to admit a pure $(1,2)$-symmetric extension, M must be a rank one matrix given by

$$\begin{aligned} M &= \vec{v}\vec{v}^\dagger \\ v_k &= e^{i\phi_k}. \end{aligned} \tag{4.17}$$

A more general test can be formulated by considering M as an adjacency matrix of a directed graph, with undefined elements representing the absence of an edge. We can then define a multiplicative traversal of a path between two vertices i and j as the product of the weights of every directed edge in the path. If the multiplicative traversal between every pair of vertices is path independent, then ρ_{AB} has a pure 2-symmetric extension. See section 6.4 for how this construction relates to unique determination, and see appendix A.3 for an algorithm employing this principle.

4.6 Spectral Insufficiency

Unlike the 2 qubit case, the general condition for pure $(1, 2)$-symmetric extension presented here requires more information about the state than simply its eigenvalues. Given that there exists a purely spectral condition for both the 2-qubit pure $(1, 2)$-symmetric extension, as well as 2-qubit mixed $(1, 2)$-symmetric extension, it bears exploring whether purely spectral conditions are possible for higher dimensions.

Indeed it has been demonstrated [25] that although the eigenvalue condition $\lambda_{AB} = \lambda_B$ is a necessary and sufficient condition for 2-qubit pure $(1, 2)$-symmetric extension, it is only a necessary condition for higher dimensional systems. This was done by finding states with no pure $(1, 2)$-symmetric extension which satisfy this condition. However these examples did not consider the spectrum of the A marginal. Here I demonstrate that no general test can exist which employs solely the eigenvalues λ_A, λ_B and λ_{AB}. This is done by showing that in every dimension greater than 2×2, a counterexample can be constructed where two states, one with a pure $(1, 2)$-symmetric extension and one without a pure $(1, 2)$-symmetric extension both have the same spectra for all marginals. It suffices to supply counterexamples in both the 2×3 case, and the 3×2 case, since they can be embedded into any higher dimensional cases.

4.6.1 2×3 case

Consider the state $|\psi_{233}\rangle \in \mathbb{H}_A \otimes \mathbb{H}_B \otimes \mathbb{H}_C = \mathbb{C}^2 \otimes \mathbb{C}^3 \otimes \mathbb{C}^3$ given by equation 4.2. Consider additionally the state $|\phi_{233}\rangle \in \mathbb{H}_A \otimes \mathbb{H}_B \otimes \mathbb{H}_C = \mathbb{C}^2 \otimes \mathbb{C}^3 \otimes \mathbb{C}^3$ given by

$$\begin{aligned}|\phi_{233}\rangle =& \frac{1}{2}(|000\rangle + |011\rangle + \sqrt{4s(1-s)}(|102\rangle + |120\rangle) \\ &+ \sqrt{1-4s(1-s)}(|101\rangle + |110\rangle)) \ , \ s \neq 1/2. \end{aligned} \tag{4.18}$$

It is known that the reduced density matrix $\rho_{23} = \mathrm{Tr}_C[\psi_{233}]$ admits no pure $(1,2)$-symmetric extension. This can be most easily observed by constructing its M matrix as

$$M[\rho_{23}] = \begin{pmatrix} \frac{0}{0} & \frac{0}{0} & 0 \\ \frac{0}{0} & \frac{0}{0} & 0 \\ 0 & 0 & \frac{0}{0} \end{pmatrix}. \tag{4.19}$$

We can see immediately that some terms are not roots of unity, which implies that this state has no pure $(1,2)$-symmetric extension.

Conversely, the reduced density matrix $\sigma_{23} = \mathrm{Tr}_C[\phi_{233}]$ does admit a pure $(1,2)$-symmetric extension. This is known simply by observing that $|\phi_{233}\rangle$ is symmetric. However it is illustrative to consider its M matrix:

$$M[\sigma_{23}] = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}. \tag{4.20}$$

This is a rank 1 matrix $M[\sigma_{23}] = v \cdot v^\dagger$ with eigenvector $v = (\ 1,1,1\ )$. This indicates that the state has a pure $(1,2)$-symmetric extension.

Finally, the eigenvalues of the marginals of both ρ_{23} and σ_{23} are $\lambda_A = \left\{\frac{1}{2}, \frac{1}{2}\right\}$,$\lambda_B = \left\{\frac{1-s}{2}, \frac{s}{2}, \frac{1}{2}\right\}$ and $\lambda_{AB} = \left\{0, 0, 0, \frac{1-s}{2}, \frac{s}{2}, \frac{1}{2}\right\}$. Since these two states share eigenvalues, but one has a pure $(1,2)$-symmetric extension and the other does not, we can conclude that for the 2×3 case the spectrum is not sufficient to test for pure $(1,2)$-symmetric extendibility.

4.6.2 3×2 case

Consider the states $|\psi_{322}\rangle, |\phi_{322}\rangle \in \mathbb{H}_A \otimes \mathbb{H}_B \otimes \mathbb{H}_C = \mathbb{C}^3 \otimes \mathbb{C}^2 \otimes \mathbb{C}^2$

$$|\psi_{322}\rangle = \sqrt{1-4s}|000\rangle + \sqrt{s}(|101\rangle + |110\rangle) + \sqrt{2s}|211\rangle \tag{4.21}$$

$$|\phi_{322}\rangle = \sqrt{1-5s}|000\rangle + \sqrt{2s}(|101\rangle + |210\rangle) + \sqrt{s}|011\rangle \tag{4.22}$$

$$s \neq 1/6, s \leq 1/5$$

the reduced density matrix $\rho_{32} = \mathrm{Tr}_C[\psi_{233}]$ is not symmetric extendible, while the reduced density matrix $\sigma_{32} = \mathrm{Tr}_C[\phi_{233}]$ is pure $(1,2)$-symmetric extendible. We can see this by examining the M matrices of ρ_{32} and ρ_{23} given by

$$M[\rho_{32}] = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, M[\sigma_{32}] = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}. \tag{4.23}$$

Finally, the eigenvalues of both ρ_{32} and σ_{32} are $\lambda_A = \{2s, 2s, 1-4s\}$,$\lambda_B = \{3s, 1-3s\}$ and $\lambda_{AB} = \{0, 0, 0, 0, 3s, 1-3s\}$.

By similar reasoning to the 2×3 case we can conclude that for the 3×2 case the spectrum is not sufficient to test for pure $(1,2)$-symmetric extendibility.

In the case of $N \times M$, $N > 2$ and $M > 2$, either of the above counterexamples suffice to show that the spectrum is not sufficient to test for pure $(1,2)$-symmetric extensions. Thus the spectrum is insufficient for all dimensions greater than 2×2.

4.7 Concluding Remarks

One of the primary motivations for characterizing the pure symmetric extendible states is that pure symmetric extendibility is a necessary condition for a state to be an extremal point on a set of symmetric extendible states. However it is not a sufficient condition. A sufficient condition can be presented in terms of uniqueness. In the next chapter we will explore the distinction between being uniquely determined among pure states and uniquely determined among mixed states. Finally, in chapter 6 we will apply this distinction to the question of extremality on the set of symmetric extendible states and present some significant progress in understanding when a pure symmetric extendible state is extremal.

Chapter 5

Unique Determination of Pure States and Mixed States

> [...]when you have eliminated the impossible, whatever remains, however improbable, must be the truth[...]
>
> Sir Arthur Conan Doyle *The Sign of the Four, 1890*

5.1 Introduction

As we've seen in the cases of both the ground states of local Hamiltonians and the symmetric extendibility problem, when presented with a quantum marginal problem it is sometimes insufficient to consider only the existence of a solution. It can often be useful to also know whether the solution is unique.

Given that the partial trace maps from a very large space to what is typically a dramatically smaller space, it would seem that under most circumstances the pre-image of a collection of marginals would contain more than one state, and that uniqueness would be rare. However the quantum landscape is expansive, and there are a great deal of instances of uniqueness in the quantum marginal problem. In fact under some circumstances uniqueness is the rule instead of the exception.

In this chapter we explore some cases of uniqueness in the quantum marginal problem. In particular we will consider the important distinction between a state

being uniquely determined among pure states and uniquely determined among mixed states. Finally I will present a novel proof demonstrating that being uniquely determined among pure states does not imply being uniquely determined among mixed states. I will do this by providing a counterexample which is the first known case of a state which is uniquely determined among pure states but not uniquely determined among mixed states by its marginals. Up to this point no known examples of this type existed, and the useful conjecture that uniqueness among pure states implies uniqueness among mixed states remained possible.

5.2 Definitions

Given a convex set of quantum states Γ, and quantum state $w \in \Gamma$, any other state $w' \in \Gamma$ is said to be a *K-imposter* of w if both states share the same K-local marginals. If a Hilbert space is given, and unless otherwise specified, Γ is assumed to be the full set of quantum states associated with that Hilbert space.

A quantum state $w \in \Gamma$ is said to be *K-uniquely determined among all states (K-UDA)* if there do not exist any K-imposters of w.

An extremal quantum state $w \in Ext(\Gamma)$ is said to be *K-uniquely determined among extremal states (K-UDE)* if there do not exist any extremal K-imposters of w.

If all of the extremal points of Γ are pure states, then the K-UDE states are said to be *K-uniquely determined among pure states (K-UDP).*

Note that K-UDA implies K-UDP. But the converse is not necessarily true.

For an illustration of the distinction between UDP and UDA, please see figure 6.2.

5.3 Known Results

Here I will review some known results regarding the uniqueness of quantum states.

For the sake of notational ease, let us define the pattern $K_2 = \{\{A, B\}, \{B, C\}\}$, and let $d_x = \dim(\mathbb{H}_x)$.

Almost every pure state of 3 qubits is K_2-UDA [38]. The only states that are not are those that are locally equivalent to $a|000\rangle + b|111\rangle$ which are neither K_2-UDA nor K_2-UDP. Consequently, in the case of 3 qubits, UDP implies UDA and what's more UDA is very common.

The commonness of UDA extends further. It has been shown that a generic tripartite pure state $|\psi\rangle \in \mathbb{H}_A \otimes \mathbb{H}_B \otimes \mathbb{H}_C$ with $d_A \geq d_B + d_C - 1$[39] is almost always K_2-UDA. A corollary is that a generic n-partite pure state $|\psi\rangle \in \mathbb{H}^{\otimes n}$ is $(\frac{2n}{3} + \frac{1}{3})$-UDA [39]. The former result has been extended such that d_A need only be greater than $\min(d_B, d_C)$[40]. A less trivial corollary of this extension is that almost every tripartite state with rank $\lfloor \frac{d_A}{d_C} \rfloor$ is K_2-UDA [40].

Furthermore, almost every tripartite pure state is K_2-UDP [41]. However despite instances where almost every state is UDP and almost every state is UDA, this does not necessarily imply that for those cases UDP implies UDA, there may be non-general states for which this does not hold.

Indeed, many of these proofs are for generic states. It is not clear that the conclusions made for generic states continue to apply for the purposes of characterizing for example symmetric states. For instance, I can demonstrate in appendix A.2 that the argument presented in [39] fails when constrained to symmetric states.

So far it is only known that UDP implies UDA for three qubit states. There does however exist a sufficient condition for UDP to imply UDA.

For a given set of quantum states $\Gamma \subset \Omega$, and a complete set of K-local observables A. If there exists a compact group G of affine automorphisms on Γ whose fixed point set is $\Gamma \cup \langle A \rangle$ where $\langle A \rangle$ denotes the real linear span of A, then K-UDP implies K-UDA [40]. In fact this theorem generalizes to general observables, not just local ones. But that goes beyond the scope of this thesis.

5.4 UDP does not imply UDA in General

It is interesting to note that in the examples outlined, whenever UDP is generic, UDA is also generic. This leads one to speculate that perhaps there is some geometric conspiracy taking place in the spectrahedron to ensure that UDP implies UDA. This

is not an unreasonable conjecture, as the spectrahedron is a highly structured object, and the local subspaces in which we are considering projections are very particular subspaces. However this turns out not to be true.

In this section I will present a family of states which are UDP but not UDA. These are the first known examples of such states and they demonstrate that in general UDP does not imply UDA. This section is largely a reproduction of previously published work [42].

We will be considering the class of 4 qubit bosonic states

$$|\psi_S\rangle = c_0|w_0\rangle + c_2|w_2\rangle + c_4|w_4\rangle \in (\mathbb{C}^2)^{\otimes 4}, \tag{5.1}$$

where

$$\begin{aligned}
|w_0\rangle =& |0000\rangle, \\
|w_2\rangle =& \frac{1}{\sqrt{6}}\left(|1100\rangle + |1010\rangle + |1001\rangle + |0110\rangle + |0101\rangle + |0011\rangle\right), \\
|w_4\rangle =& |1111\rangle,
\end{aligned}$$

and $c_i \in \mathbb{R}$.

For a given state of this type we will concern ourselves with its 2-local marginals, which, due to the symmetry of these states, will all have the same reduced density matrix $\rho_2 \in B((\mathbb{C}^2)^{\otimes 2})$.

A brief outline of the construction is as follows. I will begin by characterizing a region of values of c_0, c_2 and c_4 for which $|\psi_S\rangle$ is 2-UDP. Then I will characterize a region of values of c_0, c_2 and c_4 for which ρ_2 is separable and can be written as

$$\rho_2 = \sum_i p_i \chi^{\otimes 2}\ , \chi \in B(\mathbb{C}^2).$$

With such a decomposition, it is straightforward to see that ψ_S cannot be 2-UDA by noting that the construction

$$\rho_4 = \sum_i p_i \chi^{\otimes 4}$$

is a 2-imposter of ψ_S. Equipped with two regions, one for which $|\psi_S\rangle$ is 2-UDP, and the other for which $|\psi_S\rangle$ is not 2-UDA, we may ask if they overlap. If they do, then the space where they overlap contains states which are 2-UDP but not 2-UDA, concluding the construction. With that being said, let us proceed.

5.4.1 Region of 2-UDP States

I shall first show that almost all 4-qubit pure symmetric states of the form

$$|\psi_S\rangle = c_0|w_0\rangle + c_2|w_2\rangle + c_4|w_4\rangle, \tag{5.2}$$

for which $c_i \in \mathbb{R}$, are uniquely determined among all pure bosonic states by their 2-RDMs. In particular, I will show that

Lemma 5.4.1. *$|\psi_S\rangle = c_0|w_0\rangle + c_2|w_2\rangle + c_4|w_4\rangle$ is uniquely determined among all pure bosonic states via its 2-local reduced density matrix ρ_2 if $c_i \in \mathbb{R}$ and ρ_2 has three distinct eigenvalues on the symmetric subspace and $c_2 \neq 0$.*

Proof. Consider the Schmidt decomposition of $|\psi_S\rangle$ between the 1, 2 and 3, 4 Hilbert spaces. Noting that it is symmetric under the exchange of the 1, 2 and 3, 4 Hilbert spaces, it is straightforward to see that the Schmidt decomposition must take the form

$$|\psi_S\rangle = \sum_{i=1}^{3} \sqrt{\lambda_i}|\mu_i\rangle|\mu_i\rangle. \tag{5.3}$$

By examining the Schmidt decomposition of $|\psi_S\rangle$, we note that $\frac{1}{\sqrt{2}}(|10\rangle + |01\rangle)$ is always an eigenvector of the 2-RDMs of $|\psi_S\rangle$. Without loss of generality, we assume $|\mu_1\rangle = \frac{1}{\sqrt{2}}(|10\rangle + |01\rangle)$. Solving for $|\mu_2\rangle$ and $|\mu_3\rangle$ amounts to solving the eigenvector problem of a real symmetric matrix, therefore without loss of generality $|\mu_2\rangle = a|00\rangle + b|11\rangle$, and $|\mu_3\rangle = b|00\rangle - a|11\rangle$, $a, b \in \mathbb{R}$.

Using the assumption that the eigenvalues λ_i are non-degenerate, any state which shares the same 1,2 and 3,4 RDMs of ψ_S must take the form

$$|\phi_S(\phi_2, \phi_3)\rangle = \sqrt{\lambda_1}|\mu_1\rangle|\mu_1\rangle + \sqrt{\lambda_2}e^{i\phi_2}|\mu_2\rangle|\mu_2\rangle + \sqrt{\lambda_3}e^{i\phi_3}|\mu_3\rangle|\mu_3\rangle. \tag{5.4}$$

Expanding the $|\mu_i\rangle$ terms it is straightforward to show that

$$|\phi_S(\phi_2,\phi_3)\rangle = c_0(\phi_2,\phi_3)|w_0\rangle + \sqrt{\frac{3\lambda_1}{2}}|w_2\rangle + c_4(\phi_2,\phi_3)|w_4\rangle + f(\phi_2,\phi_3)(|0011\rangle + |1100\rangle), \tag{5.5}$$

$$c_0(\phi_2,\phi_3) = \sqrt{\lambda_2}e^{i\phi_2}a^2 + \sqrt{\lambda_3}e^{i\phi_3}b^2, \tag{5.6}$$

$$c_4(\phi_2,\phi_3) = \sqrt{\lambda_2}e^{i\phi_2}b^2 + \sqrt{\lambda_3}e^{i\phi_3}a^2, \tag{5.7}$$

$$f(\phi_2,\phi_3) = \sqrt{\lambda_2}e^{i\phi_2}ab - \sqrt{\lambda_3}e^{i\phi_3}ab - \frac{\sqrt{\lambda_1}}{2}. \tag{5.8}$$

In order for $|\phi_S(\phi_2,\phi_3)\rangle$ to be totally symmetric $f(\phi_2,\phi_3) = 0$. By virtue of $|\phi_S(0,0)\rangle = |\psi_S\rangle$, it must be the case that $f(0,0) = 0$. To show that $|\psi_S\rangle$ is UDP it suffices to show that $f(\phi_2,\phi_3) \neq 0$, $\{\phi_2,\phi_3\} \neq \{0,0\}$ such that there can be no other totally symmetric states which share the same RDMs as $|\psi_S\rangle$. This is equivalent to asking under what conditions does the equation

$$e^{i\phi_2}\sqrt{\lambda_2}ab - e^{i\phi_3}\sqrt{\lambda_3}ab = \sqrt{\lambda_2}ab - \sqrt{\lambda_3}ab = \sqrt{\lambda_1}/2 \tag{5.9}$$

have a single solution in $\{\phi_2,\phi_3\}$.

We can consider the set of points $e^{i\phi_2}\sqrt{\lambda_2}ab$ and $\sqrt{\lambda_1}/2 + e^{i\phi_3}\sqrt{\lambda_3}ab$ to be circles with radii $|\sqrt{\lambda_2}ab|$ and $|\sqrt{\lambda_3}ab|$, as illustrated in figure 5.1. Any solutions to equation 5.9 will be intersections of those two circles.

It is clear that unless the two circles totally overlap, they only intersect at one point, namely where $\phi_2 = \phi_3 = 0$. The two circles will only totally overlap when $\lambda_1 = 0$. Therefore if the eigenvalues of the 2-RDM of $|\psi_S\rangle$ are non degenerate, and $c_2 \neq 0$ then the state $|\psi_S\rangle$ is UDP. Note that the degeneracy of the eigenvalues does not necessarily imply $c_2 = 0$, as equation 5.9 was derived under the assumption of non-degeneracy.

□

I should like to now present a proof that the pure state ψ_S is generally UDP, not just among bosonic states.

Lemma 5.4.2. *Any pure state which is uniquely determined among all bosonic pure states is also uniquely determined among all pure states via its 2-RDMs.*

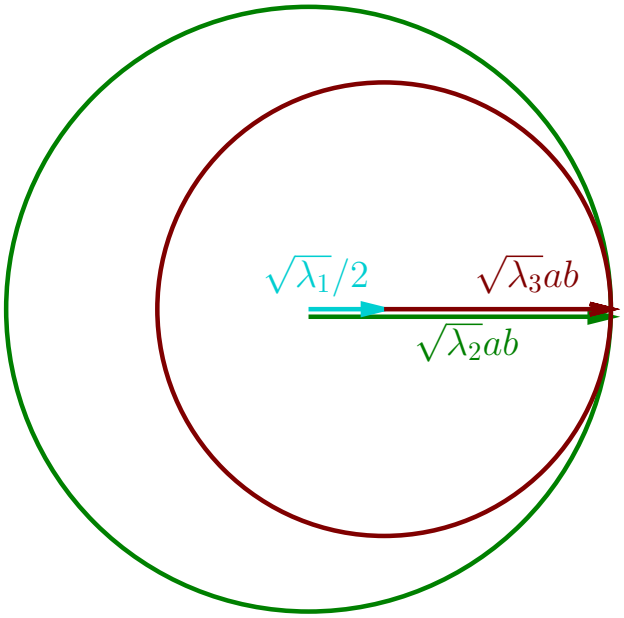


Figure 5.1: The set of points corresponding to $e^{i\phi_2}\sqrt{\lambda_2}ab$ (green) and $\sqrt{\lambda_1}/2 + e^{i\phi_3}\sqrt{\lambda_3}ab$ (red) under the constraint of equation 5.9

Proof. Consider a multipartite state $w_{1,2,\cdots,n}$ with subsystems 1 through n. Suppose that every $\{i,j\}$-local marginal $w_{i,j}$ of $w_{1,2,\cdots,n}$ is bosonic under the exchange of i and j, that is $w_{i,j}(S_{i,j}x) = w_{i,j}(x)\ \forall x \in B(\mathbb{H}_i \otimes \mathbb{H}_j)$. We can construct the antisymmetric projector $A_{i,j} = \mathbb{1} - S_{i,j}$ and note that $w_{i,j}(A_{i,j}) = 0$. Since $w_{1,2,\cdots n}(x) = w_{i,j}(x)\ \forall x \in B(\mathbb{H}_i \otimes \mathbb{H}_j)$ it follows that $w_{1,2,\cdots n}(A_{i,j}) = 0$ for all i and j. Therefore $w_{1,2,\cdots n}$ has a density matrix with support only on the totally symmetric Hilbert space and $w_{1,2,\cdots n}$ is bosonic.

Let the bosonic state $|\varphi\rangle$ be uniquely determined among all bosonic pure states via its 2-RDMs. Suppose $|\chi\rangle$ has the same 2-RDM as $|\varphi\rangle$. The above argument implies $|\chi\rangle$ has to be bosonic. Therefore, $|\chi\rangle$ has to be $|\varphi\rangle$. Thus, $|\varphi\rangle$ is 2-UDP in general.

□

Putting together lemmas 5.4.1 and 5.4.2, we find that

Theorem 5.4.3. *$|\psi_S\rangle = c_0|w_0\rangle + c_2|w_2\rangle + c_4|w_4\rangle$ is 2-UDP if $c_i \in \mathbb{R}$, $c_2 \neq 0$, $c_0 \neq -c_4$*

and $(c_2^2/2 - c_0^2)(c_2^2/2 - c_4^2) \neq c_2^2(c_0 + c_4)^2/3$.

Proof. The 2-local reduced density matrix of $|\psi_S\rangle$ is

$$\rho_2 = \begin{pmatrix} c_0^2 + \frac{c_2^2}{6} & 0 & 0 & \frac{c_0 c_2}{\sqrt{6}} + \frac{c_4 c_2}{\sqrt{6}} \\ 0 & \frac{c_2^2}{3} & \frac{c_2^2}{3} & 0 \\ 0 & \frac{c_2^2}{3} & \frac{c_2^2}{3} & 0 \\ \frac{c_0 c_2}{\sqrt{6}} + \frac{c_4 c_2}{\sqrt{6}} & 0 & 0 & \frac{c_2^2}{6} + c_4^2 \end{pmatrix}.$$

Explicit calculations of the eigenvalues of ρ_2 according to the constraints of lemma 5.4.1 give the constraints on c_0, c_2, and c_4 expressed in the theorem. □

5.4.2 Region of non 2-UDA States

Now I will present a region where $|\psi_S\rangle = c_0|w_0\rangle + c_2|w_2\rangle + c_4|w_4\rangle$ is not UDA. We observe that if the 2-RDM ρ_2 of $|\psi_S\rangle$ is separable, then it can be expressed as $\rho_2 = \sum_i p_i \chi_i^{\otimes 2}$. Then we can construct a state $\rho_4 = \sum_i p_i \chi_i^{\otimes 4}$ which has the same 2-RDMs as $|\psi_S\rangle$. Therefore, if $|\psi_S\rangle$ has a separable 2-RDM whose rank is not 1, then it is not UDA by its 2-RDMs.

A 2-qubit state is separable if it has a positive partial transpose (PPT) [2]. Direct calculation shows that a 2-RDM of $|\psi\rangle$,

$$\rho_2 = \begin{pmatrix} c_0^2 + \frac{c_2^2}{6} & 0 & 0 & \frac{c_0 c_2}{\sqrt{6}} + \frac{c_4 c_2}{\sqrt{6}} \\ 0 & \frac{c_2^2}{3} & \frac{c_2^2}{3} & 0 \\ 0 & \frac{c_2^2}{3} & \frac{c_2^2}{3} & 0 \\ \frac{c_0 c_2}{\sqrt{6}} + \frac{c_4 c_2}{\sqrt{6}} & 0 & 0 & \frac{c_2^2}{6} + c_4^2 \end{pmatrix},$$

is PPT if and only if

$$\begin{aligned} c_2^4/9 &\leq (c_0^2 + c_2^2/6)(c_4^2 + c_2^2/6), \\ \frac{2}{3} c_2^2 &\geq (c_0 + c_4)^2. \end{aligned} \tag{5.10}$$

Finally, ρ_2 is not rank 1 for $(c_0, c_2, c_4) \neq (\pm 1, 0, 0), (0, 0, \pm 1)$.

The overlap of the two regions presented here, one for which ψ_S is 2-UDP and the other for which ψ_S is not 2-UDA is illustrated in Fig. 5.4.2. Given that we are

considering a unit length vector of three real parameters (c_0, c_2,c_4), we can map our parameter space to the surface of a sphere. The green region illustrates the domain where the 2-RDMs of $|\psi_S\rangle$ are separable, and thus UDA. The red curves indicate where $|\psi_S\rangle$ fails to be UDP. Thus the green domain not intersecting the red curves is where $|\psi_S\rangle$ is UDP but not UDA.

5.4.3 The separable decomposition

For the sake of completeness, the reader may be interested in a concrete construction of the particular imposter state ρ_4. In this section I will construct an explicit separable decomposition of $\rho_2 = \sum_i p_i \chi_i^{\otimes 2}$ of $|\psi_S\rangle$ [43], retrieving the sets $\{p_i\}$ and $\{\chi_i\}$ and consequently the construction $\rho_4 = \sum_i p_i \chi_i^{\otimes 4}$.

Consider the 2-RDM of our state $|\psi_S\rangle$,

$$\rho_2 = \begin{pmatrix} c_0^2 + \frac{c_2^2}{6} & 0 & 0 & \frac{c_0 c_2}{\sqrt{6}} + \frac{c_4 c_2}{\sqrt{6}} \\ 0 & \frac{c_2^2}{3} & \frac{c_2^2}{3} & 0 \\ 0 & \frac{c_2^2}{3} & \frac{c_2^2}{3} & 0 \\ \frac{c_0 c_2}{\sqrt{6}} + \frac{c_4 c_2}{\sqrt{6}} & 0 & 0 & \frac{c_2^2}{6} + c_4^2 \end{pmatrix}.$$

To simplify notation we can define the variables a, b, c, d such that:

$$\rho_2 = \begin{pmatrix} a & 0 & 0 & c \\ 0 & d & d & 0 \\ 0 & d & d & 0 \\ c & 0 & 0 & b \end{pmatrix}.$$

ρ_2 can then be expressed as a Bloch vector expansion:

$$\rho_2 = \frac{1}{4}\mathbb{1} \otimes \mathbb{1} + \frac{c+d}{2}\sigma_x \otimes \sigma_x + \frac{d-c}{2}\sigma_y \otimes \sigma_y + \frac{a+b-2d}{4}\sigma_z \otimes \sigma_z + \frac{a-b}{4}\left(\sigma_z \otimes \mathbb{1} + \mathbb{1} \otimes \sigma_z\right).$$

Given that ρ_2 is PPT, we know that

$$a, b, d \geq 0, ab \geq c^2, ab \geq d^2, d \geq |c|.$$

Consider now the following transformation:

$$\tilde{\rho_2} = (V \otimes V)\, \rho_2\, (V \otimes V)^\dagger, V = \begin{pmatrix} e^\epsilon & 0 \\ 0 & e^{-\epsilon} \end{pmatrix}.$$

We can again write the Bloch vector expansion

$$\begin{aligned}\tilde{\rho_2} =& \frac{ae^{4\epsilon} + 2d + be^{-4\epsilon}}{4}\mathbb{1}\otimes\mathbb{1} + \frac{c+d}{2}\sigma_x\otimes\sigma_x + \frac{d-c}{2}\sigma_y\otimes\sigma_y \\ &+ \frac{ae^{4\epsilon} - 2d + be^{-4\epsilon}}{4}\sigma_z\otimes\sigma_z + \frac{ae^{4\epsilon} - be^{-4\epsilon}}{4}\left(\sigma_z\otimes\mathbb{1} + \mathbb{1}\otimes\sigma_z\right).\end{aligned}$$

Choose ϵ such that $e^{4\epsilon} = \sqrt{\frac{b}{a}}$, then

$$\tilde{\rho_2} = \frac{1}{4}\left(d_0\mathbb{1}\otimes\mathbb{1} + d_x\sigma_x\otimes\sigma_x + d_y\sigma_y\otimes\sigma_y + d_z\sigma_z\otimes\sigma_z,\right)$$

where

$$\begin{aligned}d_0 = 2\sqrt{ab} + 2d,\ d_x = 2c + 2d,\\ d_y = 2d - 2c,\ d_z = 2\sqrt{ab} - 2d,\end{aligned}$$

By noticing $d_0 = d_x + d_y + d_z$, and $d_x, d_y, d_z \geq 0$, we have the following equality

$$\tilde{\rho_2} = \sum_{k\in(x,y,z)}\frac{d_k}{4}(\mathbb{1}\otimes\mathbb{1} + \sigma_k\otimes\sigma_k) = \sum_{k\in(x,y,z)}\frac{d_k}{8}[(\mathbb{1}+\sigma_k)\otimes(\mathbb{1}+\sigma_k) + (\mathbb{1}-\sigma_k)\otimes(\mathbb{1}-\sigma_k)].$$

We can now perform the inverse map to retrieve our original state, noticing that our map preserves the manifestly separable structure of our state

$$\begin{aligned}\rho_2 &= \left(V^{-1}\otimes V^{-1}\right)\tilde{\rho}\left(V^{-1}\otimes V^{-1}\right)^\dagger \\ &= \sum_{k\in(x,y,z)}\frac{d_k}{8}\left(V^{-1}\otimes V^{-1}\right)[(\mathbb{1}+\sigma_k)\otimes(\mathbb{1}+\sigma_k) + (\mathbb{1}-\sigma_k)\otimes(\mathbb{1}-\sigma_k)]\left(V^{-1}\otimes V^{-1}\right)^\dagger \\ &= \sum_{k\in(x,y,z)}\frac{d_k}{8}(V^{-2} + V^{-1}\sigma_k V^{-1})^{\otimes 2} + \sum_{k\in(x,y,z)}\frac{d_k}{8}(V^{-2} - V^{-1}\sigma_k V^{-1})^{\otimes 2}.\end{aligned}$$

Noting that $V^{-2} + V^{-1}\sigma_k V^{-1}$ and $V^{-2} - V^{-1}\sigma_k V^{-1}$ are non-normalized pure states we can retrieve the separable construction of

$$\rho_2 = \sum_k p_k^+(\chi_k^+)^{\otimes 2} + \sum_k p_k^-(\chi_k^-)^{\otimes 2}$$

with

$$\begin{aligned}p_k^\pm &= \frac{d_k}{8}\,\mathrm{Tr}(V^{-2}\pm V^{-1}\sigma_k V^{-1})^2, \\ \chi_k^\pm &= \frac{V^{-2}\pm V^{-1}\sigma_k V^{-1}}{\mathrm{Tr}(V^{-2}\pm V^{-1}\sigma_k V^{-1})},\end{aligned}$$

and we can construct the imposter state

$$\rho_4 = \sum_k p_k^+ (\chi_k^+)^{\otimes 4} + \sum_k p_k^- (\chi_k^-)^{\otimes 4}.$$

5.4.4 Experimental Instantiation

Thanks to my colleagues at the IQC, states ψ of the form given in theorem 5.4.3 have been prepared in the laboratory as pseudo-pure states of four carbon-13 atoms in a molecular substrate[42]. Full state tomography of the carbon atoms can be achieved by employing NMR technology, thus verifying the correct preparation of quantum states as close to ψ as possible. Furthermore, state tomography of the 2-particle marginals can also be achieved. In a similar fashion the imposter state ρ_4 described in the previous section can also be faithfully prepared, and we can observe that it shares the same 2-particle marginals as ψ.

One note to make is that no guarantee has been made in this work on the numerical stability of the UDP result given in theorem 5.4.3 when c_i moves infinitesimally into the complex numbers. It would be nice to know if this result holds in this regime, so that we could be certain that the states experimentally prepared are indeed UDP states, and not merely arbitrarily close to UDP states.

5.4.5 Not All K-UDP States are Unique Ground States of K-Local Hamiltonians

An interesting corollary of the above counterexample is that there exist pure states that are uniquely determined by their K-local marginals, but which are not unique ground states of any K-local Hamiltonians. Recalling that the ground states of K-local Hamiltonians are K-correlated, we can note that if a pure state is K-UDP but not K-UDA, then it is not a K-correlated face, and consequently is not the unique ground state of a K-local Hamiltonian.

5.5 Concluding Remarks

It is unfortunate that UDP does not imply UDA in general, as it would simplify the analysis of quantum many body systems. As I shall demonstrate in the next chapter, it would be of particular use in characterizing the extreme points of symmetric extendible states. However the proof demonstrated here does not preclude the possibility of UDP implying UDA under certain circumstances. Indeed it remains open whether UDP implies UDA for the circumstances I will consider in the next chapter.

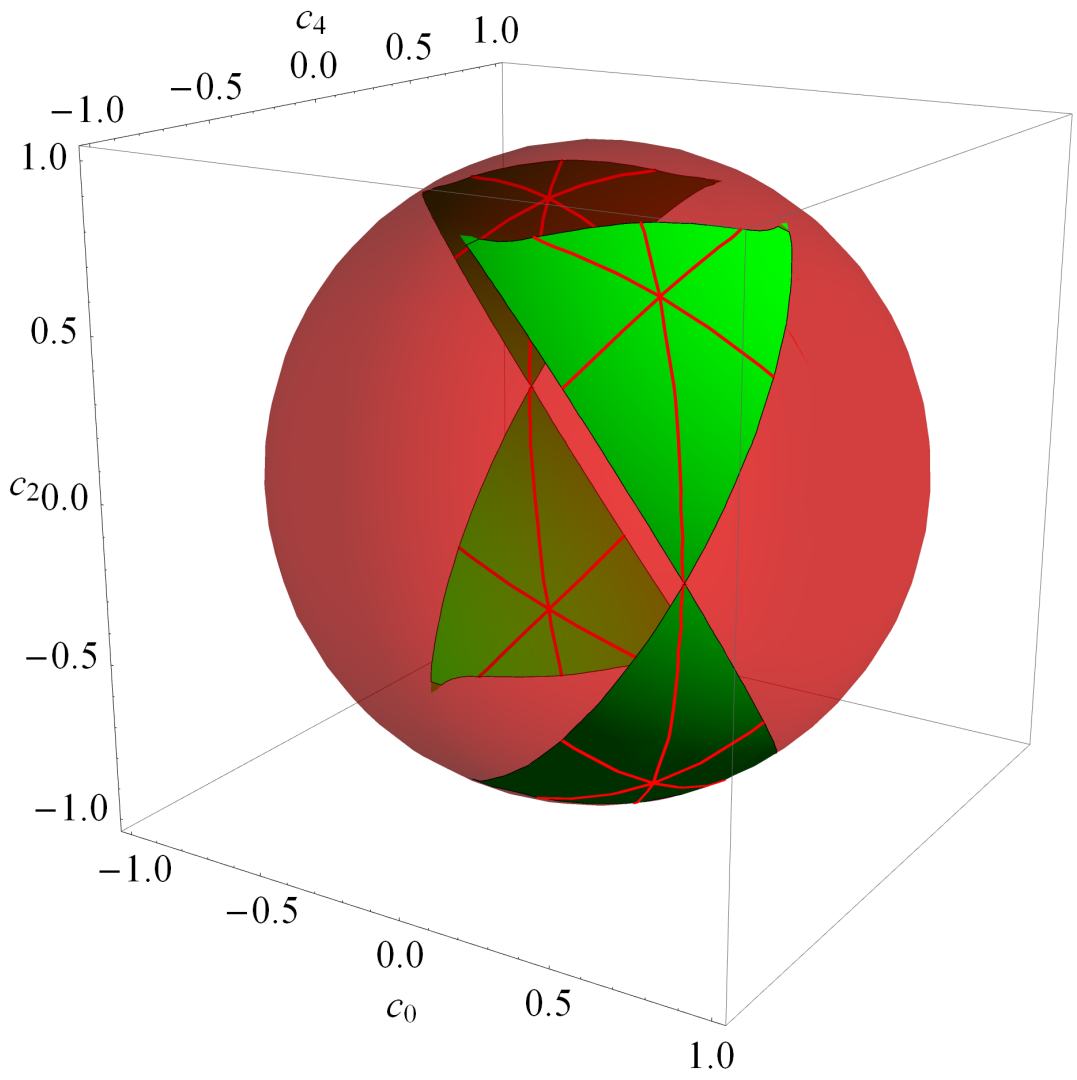


Figure 5.2: The parameter space of $|\psi_S\rangle$. The green region is where $|\psi_S\rangle$ is UDP and not UDA, given by the inequalities in Eq. (5.10) and theorem 5.4.3. The red region is where $|\psi_S\rangle$ is not necessarily UDP or may be UDA.

Chapter 6

Unique Determination Of Pure Symmetric Extensions

6.1 Introduction

Given an understanding of the nature of uniqueness in the quantum marginal problem, I would like now to address its role in characterizing the extremal points of symmetric extendible states.

In this chapter I will explain precisely in what way uniqueness is important in characterizing extremal points. I will then proceed with a novel proof demonstrating that for 2-symmetric extendibility, all extremal points of the set of solutions admit extensions which are UDP. I will show that a corollary of this fact is that a 2-symmetric extendible state is extremal if and only if it has a pure 2-symmetric extension, and that extension is UDA. I will give a characterization of those states with UDP 2-symmetric extensions, which then begs the question, equipped with a characterization of such states, do we have a characterization of the extremal points. The answer to this question rests on whether UDP implies UDA in the case of 2-symmetric extensions, a question which I will attempt to address, but which ultimately will remain open for future work.

6.2 Definitions

Recalling the definition of a K-imposter of a quantum state from chapter 5.

A K-imposter w' of w is said to be *unfaithful* if it admits a decomposition into a convex sum of extremal states in Γ of which at least one is not a K-imposter.

A K-imposter w' of w is said to be *conspiratorial* if it does not admit a decomposition into a convex sum of extremal K-imposter states.

A K-imposter w' of w is said to be *extremely conspiratorial* if it does not admit a decomposition into a convex sum of extremal states of which at least one is a K-imposter state.

Note that every conspiratorial K-imposter is unfaithful, but not every unfaithful K-imposter is conspiratorial.

Note also that if a state has a conspiratorial K-imposter, then it must also have an extremely conspiratorial K-imposter. Consider a state w and a conspiratorial K-imposter w'. Consider a line between w and w' in Hilbert-Schmidt space. The segment of this line which is contained within Γ contains only points that are K-imposters of w. There will always be a face on Γ which the line passes through which does not contain w, to see this consider following the line away from w, through w' and then out of the set Γ. The point where the line exits Γ is such a point. Therefore the state associated with this point has no support on w, and consequently is an extremely conspiratorial K-imposter.

6.3 A Necessary and Sufficient Condition for Solution Extremality

It has been alluded to previously that unique determination plays an important role in the quantum marginal problem. Equipped with a notion of an unfaithful K-imposter, we are now in a position to understand precisely what that means. What I will present in this section is likely understood by those who have worked on these problems [25], and so is not strictly novel. However I have not seen any sufficiently

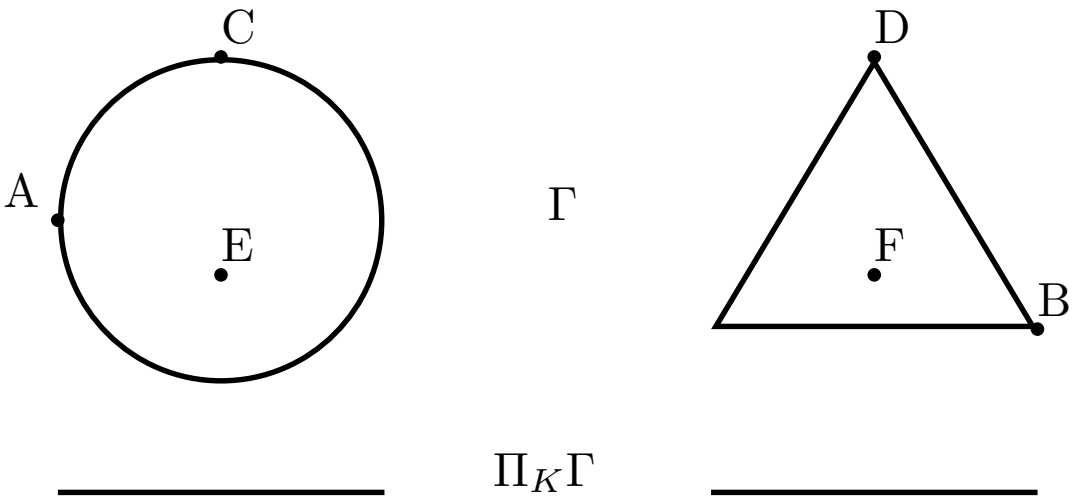


Figure 6.1: An illustration of the various uniqueness scenarios. Let the circle and the triangle represent possible subsets of the spectrahedron, and let the line beneath them represent their K-projection. Points A and B are K-UDP and K-UDA. Point C is neither K-UDP nor K-UDA. Point D is K-UDP, but not K-UDA. Point E is an unfaithful K-imposter of point C. Point F is a conspiratorial K-imposter of point D.

concrete exposition on this point that satisfies my purposes, and so I would like to do that now.

Let Ω be the spectrahedron of some quantum system and let $\Gamma \subset \Omega$ be some set of states that are of interest, for example in the case of symmetric extendibility they would be the symmetric states. Let the function $Ext(\cdot)$ denote the extremal points of a set. Finally, let Π_K be the K-projector.

Lemma 6.3.1. *If a state has an unfaithful K-imposter then its K-projection is not extremal on the set of solutions*

Proof. Let $\alpha \in \Gamma$ be an extension of $\Pi_K\alpha$. Suppose α has an unfaithful K-imposter $\beta = \sum_i p_i\beta_i^*$ with $\beta_i^* \in Ext(\Gamma)$ such that $\Pi_K\beta = \Pi_K\alpha$ and $\Pi_K\beta_i^* \neq \Pi_k\alpha$ for some i. Then $\Pi_K\alpha = \sum_i p_i\Pi_K\beta_i^*$ which implies $\Pi_K\alpha \notin Ext(\Pi_K\Gamma)$. □

Lemma 6.3.2. *If a solution α_K is extremal in the set of solutions $\Pi_K\Gamma$, then it has an extension that is extremal in Γ.*

Proof. Suppose there does not exist an extension that is extremal in Γ. Since α_K is a solution, it must have a non extremal extension $\alpha = \sum_i p_i\beta_i^*$ with $\beta_i^* \in Ext(\Gamma)$ and

$\Pi_K \alpha = \alpha_K$. For all i it must be the case that $\Pi_K \beta_i^* \neq \alpha_K$ since α_K has no extremal extensions. Therefore $\Pi_K \alpha = \alpha_K = \sum_i p_i \Pi_K \beta_I^* \notin Ext(\Pi_K \Gamma)$. □

Lemma 6.3.3. *If a solution α_K is not extremal in the set of solutions $\Pi_K \Gamma$ then it has an extension with an unfaithful K-imposter.*

Proof. Suppose α_K is not extremal, so that $\alpha_K = \sum_i p_i (\alpha_K^*)_i$ with $(\alpha_K^*)_i \in Ext(\Pi_K \Gamma)$. From lemma 6.3.2 we know there exists a family of extremal extensions $\{\alpha_i^*\}$ such that $\Pi_K \alpha_i^* = (\alpha_K^*)_i$. Therefore $\alpha_K = \sum_i p_i \Pi_K \alpha_i^* = \Pi_K \sum_i p_i \alpha_i^*$. We see that $\sum_i p_i \alpha_i^*$ is an unfaithful imposter. □

Theorem 6.3.4. *Given a quantum marginal problem, a solution is an extremal point on the set of solutions if and only if its extensions do not have any unfaithful K-imposters.*

Proof. From lemma 6.3.1 we know that if a state's K-projection is extremal on the set of solutions $\Pi_K \Gamma$, then it does not have an unfaithful K-imposter. From lemma 6.3.3 we know that if a state does not have an unfaithful K-imposter, then it's K-projection is extremal in the set of solutions. Therefore a solution is an extremal point on the set of solutions $\Pi_K \Gamma$ if and only if its extensions do not have any unfaithful K-imposters.

□

Finally we can understand how uniqueness relates to extremal points. If a state is K-UDA in Γ, it has no K-imposters, let alone any unfaithful ones. As such it is a trivial corollary that if a state is K-UDA in Γ, then its K-projection is an extremal point on the set of solutions $\Pi_K \Gamma$. However this remains a sufficient condition and not a necessary condition.

6.4 Necessary and Sufficient Condition for a UDP 2-Symmetric Extension

Returning to 2-symmetric extension, and equipped with the fact that UDA is a sufficient condition for a 2-symmetric extendible state to be extremal, we are mo-

tivated to ask, under what conditions are 2-symmetric extensions UDA? It is in general hard to determine if a state is UDA, so we shall for the moment consider under what conditions a 2-pure symmetric extension is UDP, which is a necessary condition for 2-UDA. The proof presented here is largely similar to one presented by Diosi [41] with one major difference. Diosi considers generic tripartite pure states in $\mathbb{H}_A \otimes \mathbb{H}_B \otimes \mathbb{H}_C$, and concludes that almost all of them are K_2-UDP, recalling the notation $K_2 = \{\{A, B\}, \{B, C\}\}$. Here we will account for the non-generic cases of tripartite pure states that are not K_2-UDP, and relate these to the necessary and sufficient condition for 2-pure symmetric extendibility discussed in the previous chapter.

Consider a pure symmetric state $|\psi\rangle$ which must either be bosonic $|\psi\rangle \in \mathbb{H}_A \otimes Sym(\mathbb{H}_B \otimes \mathbb{H}'_B)$ or fermionic $|\psi\rangle \in \mathbb{H}_A \otimes ASym(\mathbb{H}_B \otimes \mathbb{H}'_B)$. It admits a Schmidt decomposition

$$|\psi\rangle = \sum_i |G_i\rangle|i\rangle,$$

with $|G_i\rangle \in \mathbb{H}_A \otimes \mathbb{H}_B$ and $|i\rangle \in \mathbb{H}'_B$. The pure state $|\psi\rangle$ is a 2-pure symmetric extension of the state $\rho_{AB} = \sum_i |G_i\rangle\langle G_i|$. We can further decompose $|G_i\rangle = \sum_j |D_{ij}\rangle|j\rangle$, with $|D_{ij}\rangle = \pm|D_{ji}\rangle \in \mathbb{H}_A$ a non-normalized vector, note that this is not a Schmidt decomposition and $\pm$ indicates the bosonic or fermionic symmetry. This gives us

$$|\psi\rangle = \sum_{ij} |D_{ij}\rangle|j\rangle|i\rangle.$$

We should like to parametrize all other 2-pure symmetric extensions of ρ_{AB}.

If the nonzero eigenvalues of ρ_{AB} are non-degenerate, then all 2-pure symmetric extensions of ρ_{AB} must take the form

$$|\psi(\vec{\theta})\rangle = \sum_{ij} e^{i\theta_i}|D_{ij}\rangle|j\rangle|i\rangle,$$

with $e^{i\theta_i}|D_{ij}\rangle = \pm e^{i\theta_j}|D_{ji}\rangle = e^{i\theta_j}|D_{ij}\rangle$. This implies that for every pair i, j, $e^{i\theta_i} = e^{i\theta_j}$ or $|D_{ij}\rangle = 0$. We can visualize this as a graph with $dim(\mathbb{H}_B)$ vertices, each vertex being associated with an index value i. An edge is present between vertices i and j whenever $\langle D_{ij}|D_{ij}\rangle > 0$. We may note that the matrix M introduced in chapter 4 can be thought of as an adjacency matrix of this graph. A connected component of

a graph is any subgraph in which all vertices are connected by a path, and no other vertices outside of the subgraph are connected to any vertices in the subgraph by a path. If our graph has only 1 connected component (the whole graph) then for every pair of indices i, j a path can be found between their associated vertices. This implies that $e^{i\theta_i} = e^{i\theta_j}$ even if $|D_{ij}\rangle = 0$, and thus $|\psi\rangle$ is the only 2-pure symmetric extension of ρ_{AB}, this implies that $|\psi\rangle$ is K_2-UDP. This is a necessary and sufficient condition for being K_2-UDP, as states for which ρ_{AB} have degenerate non-zero eigenvalues are trivially not K_2-UDP. If the graph contains $n+1$ connected components, then there are n phases which are not fixed, and thus there is an n parameter family of 2-pure symmetric extensions of ρ_{AB}. An algorithm for testing whether ρ_{AB} has a UDP pure 2-symmetric extenison is given in appendix A.3.

6.5 A Pure 2-Symmetric Extension of an Extremal Solution is Always UDP

We know that extremal points on the set of symmetric extendible states always have a pure symmetric extension. It turns out that in the case of 2-symmetric extension, this pure extension is UDP. As we shall see, this is significant because it implies that 2-symmetric extendible states are extremal if and only if they have an extension that is UDA.s

Theorem 6.5.1. *If a state w_{AB} admits a pure 2-symmetric extension ψ and is extremal on the set of 2-symmetric extendible states, then ψ is UDP.*

Proof. Let $|\psi\rangle = \sum_i |G_i\rangle|i\rangle$ with $|G_i\rangle \in \mathbb{H}_A \otimes \mathbb{H}_B$, $\langle G_i|G_j\rangle = \lambda_i \delta_{ij}$ and $|i\rangle \in \mathbb{H}_{B'}$.

If $|\psi\rangle$ is not UDP in the symmetric states, then we know from the previous section that there exist a family of phases $\{\vec{\theta}\}$ which characterize all pure imposters

$$|\psi(\vec{\theta})\rangle = \sum_i^r e^{i\theta_i}|G_i\rangle|i\rangle.$$

Consider the largest set of mutually orthogonal states one could construct from the pure imposters. Let the size of this set be N_O. Consider now the largest set of linearly

independent states one could construct from the pure imposters. Let the size of this set be N_L.

Lemma 6.5.2. *If $N_L > N_O$ then there exists an unfaithful K-imposter of ψ.*

Proof. Consider a state $\sigma_{ABB'} = \sum_i^{N_L} P_i |\psi(\theta_i)\rangle\langle\psi(\theta_i)|$ where $\{|\psi(\theta_i)\rangle\}$ form a largest set of linearly independent pure K-imposters of $|\psi\rangle$. $\sigma_{ABB'}$ is rank N_L, and so admits a singular value decomposition $\sigma_{ABB'} = \sum_i^{N_L} \gamma_i |\phi_i\rangle|\phi_i\rangle$. However since $N_L > N_O$ at least one of the eigenvectors of $\sigma_{ABB'}$ must not be a pure K-imposter of $|\psi\rangle$. Therefore $\sigma_{ABB'}$ is an unfaithful K-imposter of ψ. □

Lemma 6.5.3. *If ψ is not UDP then N_L is always greater than N_O.*

Proof. Suppose ψ is not UDP. This implies there is an m parameter family of pure imposter states $\psi(\vec{\theta})$, with $1 \leq m < r$ and $r - m$ elements of every $\vec{\theta}$ are fixed to 0. Note, $m < r$ due to the single phase degree of freedom of a quantum state, without loss of generality we can set $\theta_0 = 0$.

At the very least $N_L \geq N_O$, since orthogonal states are linearly independent. So it suffices to show that given a set of mutually orthogonal pure K-imposters, one can always construct a pure K-imposter that is linearly independent to all of them.

Consider a set of N_O mutually orthogonal pure K-imposters $\{\psi(\Theta^j)\}$, indexed by j. Any pure K-imposter which is not linearly independent to $\{\psi(\vec{\Theta}^j)\}$ will take the form

$$|\psi(\vec{\Phi})\rangle = \sum_i^r e^{i\Phi_i} |G_i\rangle|i\rangle = \sum_j^{N_O} a_j(\vec{\Phi})|\psi(\vec{\Theta}^j)\rangle.$$

Expanding the orthogonal K-imposters we find that

$$|\psi(\vec{\Phi})\rangle = \sum_i^r \sum_j^{N_O} a_j(\vec{\Phi}) e^{i\Theta_i^j} |G_i\rangle|i\rangle.$$

This implies that

$$e^{i\Phi_i} = \sum_j^{N_O} a_j(\vec{\Phi}) e^{i\Theta_i^j}.$$

Noting that $\Phi_0 = \Theta_0^j = 0$ it must be the case that

$$1 = \sum_j^{N_O} a_j(\vec{\Phi}).$$

Normalization of $|\psi(\vec{\Phi})\rangle$ requires that

$$1 = \sum_j^{N_O} |a_j(\vec{\Phi})|^2,$$

which implies that $a_j(\vec{\Phi}) = \delta_{jk}$ for some constant index k, giving us that

$$e^{i\Phi_i} = e^{i\Theta_i^k}.$$

So we may ask, does there exist some $\vec{\Phi}$ such that the above equation does not hold for some i and some k? Given that there are a finite set of possible Θ_i^k but an uncountable set of possible $\vec{\Phi}$ this task is always possible. Therefore a linearly independent state can always be found.

□

Combining lemmas 6.5.3 and 6.5.2 we see that if ψ has no unfaithful K-imposters, then ψ is UDP. Since a solution is extremal if and only if its extension ψ has no K-imposters, it follows that if a solution to the 2-symmetric extension problem does not admit a UDP symmetric extension, then it is not extremal.

□

We should note that the above proof gives a necessary condition for extremality, but not a sufficient condition. Consider the following corollary.

Corollary 6.5.4. *A 2-symmetric extendible state is extremal if and only if it admits a pure UDA extension.*

Proof. If a 2-symmetric extendible states pure extension is UDA, then it is necessarily extremal.

If a 2-symmetric extendible state is extremal, then it admits a UDP extension. If the UDP extension has a K-imposter, then that K-imposter is not rank 1. Any K-imposter of a UDP state with rank greater than 1 must be unfaithful. Therefore if a symmetric extendible state is extremal, its extension must be UDA. □

As an aside, recalling section 3.2.3, an interesting consequence of corollary 6.5.4 is that all extremal 2-symmetric extendible states have extensions that are ground states of 2-local Hamiltonians.

We see then that it may be the case that a symmetric extendible state ρ admits a pure symmetric extension ψ that is UDP but not UDA, in which case ρ is not extremal. As has been demonstrated, this is a possibility. However the example presented in chapter 5 does not necessarily preclude UDP potentially implying UDA in the case of 2-symmetric extension. I shall discuss this possibility in the next section.

6.6 Does UDP imply UDA in the 2-Symmetric Extension Problem?

Despite the fact that UDP does not imply UDA in general, it is not known in general whether UDP implies UDA for symmetric states living in spaces of the form $\mathbb{C}^{d_A} \otimes sym(\mathbb{C}^{d_B} \otimes \mathbb{C}^{d_B})$ or $\mathbb{C}^{d_A} \otimes asym(\mathbb{C}^{d_B} \otimes \mathbb{C}^{d_B})$. The only known case is of three qubits ($2 \times 2 \times 2$), for which UDP implies UDA in general. The next simplest cases are $3 \times 2 \times 2$ and $2 \times 3 \times 3$ symmetric states. So it is worth exploring whether a counterexample of the type explored in section 5.4 can be found for these spaces. We should recall that generic tripartite pure states are almost always UDA by their $\{A, B\}$ and $\{A, B'\}$ marginals. Furthermore, generic tripartite pure states are almost always UDP by their $\{A, B\}$ and $\{A, B'\}$ marginals. This suggests that counterexamples might not exist. This is further evidenced by the fact that separable counterexamples of the form presented in chapter 5 are not possible for $n \times 2 \times 2$ spaces.

Theorem 6.6.1. *If a state $\rho_{AB} \in B(\mathbb{H}_A \otimes \mathbb{H}_B) = B(\mathbb{C}^n \otimes \mathbb{C}^2)$ admits a UDP $\{1, 2\}$-pure symmetric extension, then it can not be separable.*

Proof. Consider a pure symmetric state $|\psi\rangle \in \mathbb{C}^n \otimes \mathbb{C}^2 \otimes \mathbb{C}^2$ with $\rho_{AB} = \mathrm{Tr}_B(|\psi\rangle\langle\psi|)$. It is known that $\lambda(\rho_{AB}) = \lambda(\rho_B)$ where $\lambda(x)$ is the non-zero spectrum of x. It is also known that ρ_B is at most rank 2. It is known that if ρ_{AB} is separable [14], then $\lambda(\rho_{AB}) \prec \lambda(\rho_A)$, where here $\prec$ denotes majorization. It follows that $\lambda(\rho_B) \prec \lambda(\rho_A)$.

This implies that ρ_A must be rank 2 and that $|\psi\rangle \in H_{2\times2\times2} = \mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathbb{C}^2 \subset \mathbb{C}^n \otimes \mathbb{C}^2 \otimes \mathbb{C}^2$. This reduces the $n \times 2 \times 2$ case to the $2 \times 2 \times 2$ case for which it is understood that UDP implies UDA and no such separable example can be found. $\square$

This does not preclude the existence of states which are UDP but not UDA, however they cannot take the form presented in chapter 5. Unfortunately the above proof does not work for the $n \times 3 \times 3$ case. Nevertheless it has proven very difficult to construct separable counterexamples for the $n \times 3 \times 3$ case.

Chapter 7

Conclusion

The primary aim of this thesis has been to contribute to our understanding of the quantum marginal problem. I hope I have made compelling arguments for why this problem is worth exploring – not only through explicit examples of its application to questions in physics and quantum information, but also by illustrating what I think is a deep connection to the old philosophical problems of epistemology and reality exemplified by the allegory of Plato's cave.

The way I have gone about contributing to our understanding of the quantum marginal problem is by focusing on one of the simplest instances of the problem that remains open, the 2-symmetric extendibility problem. In particular, instead of attempting to solve the general 2-symmetric extendibility problem, which remains extremely difficult, I have opted to characterize the extreme points of the set of 2-symmetric extendible states.

The first step in understanding the extreme points comes in characterizing which states have a pure 2-symmetric extension. This is because all extremal 2-symmetric extendible states have a pure 2-symmetric extension. I have given a closed form necessary and sufficient condition for when a state has a 2-symmetric extension. Furthermore I have proven that no simpler condition employing only spectra is possible.

Next I have proven that a necessary and sufficient condition for a 2-symmetric extendible state to be extremal is that its pure extension be UDA. I demonstrate that it is straightforward to test for when a 2-symmetric extendible state has a UDP

pure extension, using the same construction that is employed in testing for pure symmetric extension. However this begs the question of whether UDP implies UDA.

Consequently I supply a proof that UDP in fact does not imply UDA in general. This result is significant for understanding the quantum marginal problem beyond simply characterizing the extremal points of the 2-symmetric extendible states.

Despite knowing that UDP does not imply UDA in general, the question remains open whether UDP implies UDA for pure 2-symmetric extensions. My suspicion is that the 2-symmetric extendibility problem is sufficiently constrained such that UDP does imply UDA for pure 2-symmetric extensions. I have shown that if this were the case then the extreme points of the 2-symmetric extendible states would be completely characterized by the work presented in this thesis. However further work is required to resolve this question.

Appendix A

Appendix

A.1 All states in a K-correlated space are ground states of a K-local Hamiltonian

First, it is known that the faces of Ω_K are in correspondence with the K-correlated faces of Ω, so we will refer to them to identify the K-correlated faces, noting that the K-correlated face associated with a face of Ω_K is the pre-image of said face in Ω. It is known that every exposed face of Ω_K corresponds to a K-correlated face which is the full ground state space of a K-local Hamiltonian. So it suffices to just consider non-exposed faces. Every non-exposed face intersects a hyperplane which also intersects an exposed face. Consider the convex set Ω_K and a non-exposed face V_K with preimage V in Ω. Because a convex set is the intersection of a collection of half spaces defined by hyperplanes, every face of a convex set intersects a supporting hyperplane. Consider a supporting hyperplane which intersects V_K, call it H. The intersection $U_K = \Omega_K \cap H$ must be an exposed face, with preimage U in Ω. Thus V_K shares a supporting hyperplane with an exposed face U_K.

Since H is the supporting hyperplane of an exposed face, it corresponds to a K-local Hamiltonian given by $\vec{\theta}$ such that $u.\vec{\theta} = 0 \ | \forall u \in U$. Since V_K intersects H it must also be the case the $v.\vec{\theta} = 0 \ | \forall v \in V$ and so the preimage V is also in the ground state space of a K-local Hamiltonian.

A.2 The Parts Do Not Necessarily Determine The Whole for Generic Pure Symmetric States

In Linden and Wooters paper *The Parts Determine the Whole in a Generic Pure Quantum State* [39] the argument is made that for generic tripartite pure quantum states $|\xi\rangle \in \mathbb{H}_A \otimes \mathbb{H}_B \otimes \mathbb{H}_C$ the reduced density matrices $\rho_{AB} \in B(\mathbb{H}_A \otimes \mathbb{H}_B)$ and $\rho_{AC} \in B(\mathbb{H}_A \otimes \mathbb{H}_C)$ are sufficient to uniquely determine $|\xi\rangle$ among all mixed and pure states. That is, generic $|\xi\rangle$ are $\{\{A,B\},\{A,C\}\}$-UDA. However the argument they present fails if $|\xi\rangle$ is assumed to be bosonic or fermionic over the B and C spaces. Consider the decomposition

$$|\xi\rangle = \sum_{ijk} a_{ijk}|i\rangle_A|j\rangle_B|k\rangle_C.$$

A critical step in their argument comes at equation (10) when an identity of the following form is presented (see their paper for context):

$$\sum_{l=1}^{P} a_{i1l}|e_{l1}\rangle = \sum_{r=1}^{N} a_{ir1}|f_{r1}\rangle.$$

It is important to know that $P = dim(\mathbb{H}_C)$ and $N = dim(\mathbb{H}_B)$. This equation represents a system of $dim(\mathbb{H}_A)$ homogeneous polynomial equations with $P + N - 1$ variables, one of which is $|e_{11}\rangle - |f_{11}\rangle$, and the others are $|e_{l1}\rangle, |f_{r1}\rangle,\ l \neq 1,\ r \neq 1$. The authors use the overdetermination of this system of equations to conclude that generically the only solutions are

$$|e_{11}\rangle - |f_{11}\rangle = 0,$$

$$|e_{l1}\rangle = 0, |f_{r1}\rangle = 0,\ l \neq 1,\ r \neq 1.$$

However if one assumes bosonic or fermionic symmetry, then $a_{ijk} = \pm a_{ikj}$ and instead of $P + N - 1$ variables, one instead has P variables of the form

$$|e_{l1}\rangle \mp |f_{l1}\rangle = 0.$$

So the authors argument fails to hold in this context.

A.3 Algorithm for UDP Pure Symmetric Extension

Given a bipartite quantum state $\rho_{AB} \in \mathbb{C}^{d_a} \otimes \mathbb{C}^{d_b}$ the following algorithm tests if a ρ_{AB} admits a UDP pure symmetric extension. Let λ_i denote the eigenvalues of ρ_{AB} ordered in non-increasing order with associated eigenvectors $|g_i\rangle$. Let γ_i denote the eigenvalues of $\rho_B = \mathrm{Tr}_A(\rho_{AB})$ ordered in non-increasing order with associated eigenvectors $|f_i\rangle$. Let $d = min(d_a, d_b)$.

Algorithm 1: A test for UDP pure symmetric extension. ($O(d^2)$ runtime)

Data: $|g_i\rangle, \lambda_i, |f_i\rangle, \gamma_i, d$

Result: Returns True and $|\psi\rangle$ if ρ_{AB} admits a UDP pure symmetric extension $|\psi\rangle$. Return False otherwise.

Begin
  for $i = 1$ **to** d **do**
    if $\gamma_i \neq \lambda_i$ **then return** False;
    if $i < d$ **and** $\gamma_i \neq 0$ **and** $\gamma_i == \gamma_{i+1}$ **then return** False;
  end
  for $i = 1$ **to** d **do**
    for $j = i$ **to** d **do**
      $|D_{ij}\rangle = \sqrt{\gamma_i}\langle f_j|g_i\rangle$, $|D_{ji}\rangle = \sqrt{\gamma_j}\langle f_i|g_j\rangle$;
      $L_{ij} = \langle D_{ij}|D_{ij}\rangle$, $L_{ji} = \langle D_{ji}|D_{ji}\rangle$;
      if $L_{ij} \neq L_{ji}$ **then return** False;
      if $L_{ij} \neq 0$ **then**
        $M_{ij} = \frac{\langle D_{ij}|D_{ji}\rangle}{L_{ij}}$;
        $M_{ji} = \frac{\langle D_{ji}|D_{ij}\rangle}{L_{ji}}$;
        if $M_{ij}M_{ij}^* \neq 1$ **or** $M_{ji}M_{ji}^* \neq 1$ **then return** False;
        if $M_{ij} \neq M_{ji}^*$ **then return** False;
      end
    end
  end
  continued...

```
(18)
(19)  ... continued;
(20)  for i = 1 to d do
(21)      z_i =nil
(22)  def Function DepthFirstTraverseGraphFrom (i)
(23)      for j = 1, j ≠ i to d do
(24)          if z_j == nil and L_ij ≠ 0 then
(25)              z_j = z_i M_{i,j};
(26)              DepthFirstTraverseGraphFrom(j)
(27)  z_1 = 1;
(28)  DepthFirstTraverseGraphFrom(1);
(29)  for i = 1 to d do
(30)      if z_i =nil then return False;
(31)  for i, j = 1 to d do
(32)      if L_{i,j} ≠ 0 and M_ij ≠ z_i^{-1} z_j then return False;
(33)  |ψ⟩ = Σ_i^d z_i √λ_i |g_i⟩ ⊗ |f_i⟩;
(34)  return {True, |ψ⟩}
```

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