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Quantum states, maps, measurements and entanglement

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Quantum states, maps, measurements and entanglement

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The structure of the set of density matrices, its linear transformations, generalized linear measurements, and entanglement are studied. The set of density matrices is shown to be a convex and stratified set with simplex and group symmetries. Generalized measurements for density matrices are shown to be reducible to one unitary transformation and one von Neumann measurement carried out with an ancillary system of fixed size. Linear maps of density matrices are considered and the volume of the set of maps is derived. Positive but not completely positive maps are studied in consideration of obtaining a test for entanglement in density matrices. Using the Jamiolkowski representation and Schmidt decomposition of the

map eigen matrices, several properties of these maps are shown. An algebraic approach to constructing these positive but not completely positive maps is partially formulated.

The positivity of the linear map describing the evolution of an open system and its dependence on the initial state of the system is studied. For a system that is initialized to a zero-discord state, the evolution is shown to be given by a completely positive map. In quantum process tomography, the results obtained from a open system that is initially prepared using von Neumann measurements is shown to be described by a bi-linear map, not a linear map. A method for quantum process tomography is derived for qubit bi-linear maps. The difference between preparing states for an experiment by measurement and by stochastic process is analyzed, and it is shown that the two different methods will give fundamentally different outcomes.

Contents

List of Figures

Chapter 1

Density matrices

We will begin by reviewing some fundamentals on quantum state rays and density matrices [6], as well some simple convex set theory as applicable to density matrices. We will also discuss the real vector representation of density matrices [7] to provide a foundation for later discussions.

The original research in this chapter is the derivation of the manifold of density matrices through purification and its stratified structure [2], as well as some observations about the basis simplex and associated symmetries.

1.1 From rays to matrices

In basic quantum physics, the quantum state of a particle is given by a ray (normalized vector) $|\psi\rangle$ in a complex linear vector space. Transformations on the state are given by $U|\psi\rangle$ where U is a unitary operator. Measurement expectation values are given by $\langle\psi|P|\psi\rangle$, where P is a hermitian operator with real eigenvalues (Hilbert space).

With this basic foundation, quantum physics has given us many important

and fundamental results. However state rays cannot represent the most general quantum states:

Consider a large ensemble of particles, half of the particles are in the state $|\phi\rangle$ and half are in the state $|\psi\rangle$. A measurement P on a particle state $|\phi\rangle$ has the expectation value of $\langle\phi|P|\phi\rangle$, and similarly on the particle state $|\psi\rangle$ would have the expectation value $\langle\psi|P|\psi\rangle$.

What would be the expectation value of this measurement on a random particle taken from this ensemble? Statistics tells us the expectation of this measurement should be:

$$\frac{1}{2}\langle\phi|P|\phi\rangle + \frac{1}{2}\langle\psi|P|\psi\rangle \tag{1.1}$$

The next question is what quantum state would give the same expectation value? Unfortunately it is clear that no ray can give us the needed result.

The solution is to use matrices instead of rays to describe the quantum state. The generalized state for our example is the density matrix:

$$\rho = \frac{1}{2}|\phi\rangle\langle\phi| + \frac{1}{2}|\psi\rangle\langle\psi| \tag{1.2}$$

A particle that is in a state given by the ray $|\phi\rangle$ is now given by the density matrix $|\phi\rangle\langle\phi|$. A unitary transformation U acting on the density matrix is given by $U\rho U^\dagger$. The expectation value for measurement P is $Tr[P\rho] = \sum_i \langle i|P\rho|i\rangle$, where $|i\rangle$ is a complete basis. So nothing has been changed fundamentally in the mechanics, but density matrices allow us to deal with statistical ensembles, and as we will see later, to deal with states of open systems.

Density matrices are complex hermitian matrices. They must also satisfy the

following as a probability density:

$$\begin{array}{ll} \text{Positivity:} & \langle\phi|\rho|\phi\rangle > 0 \text{ for all } |\phi\rangle \\ \text{Normalization:} & Tr[\rho] = \sum_i \langle i|\rho|i\rangle = 1 \text{ for a complete basis } |i\rangle \end{array} \tag{1.3}$$

We will often distinguish between a density matrix of the form $|\phi\rangle\langle\phi|$ as a pure state, and any density matrix that cannot be written in this simple form as a mixed state.

1.2 Convex sets and basis simplex

Density matrices form a closed set – consider an ensemble of ensembles; take 2 ensembles, one ensemble of state ρ_1 and the second ensemble of state ρ_2, and combine them. Suppose the size of ensemble 1 and ensemble 2 are p_1 and p_2 fractions of the overall ensemble respectively. A random particle taken from this overall ensemble should then have the state $p_1\rho_1 + p_2\rho_2$. It can be easily verified that this remains a complex positive hermitian matrix of unit trace.

We can see that in general any combination $\sum_i p_i\rho_i$ is a valid density matrix as long as $p_i > 0$ and $\sum_i p_i = 1$. A sum with positive coefficients that add to 1 is known as a convex sum. A convex sum has a geometrical interpretation; it is a closed set with a convex surface.

For example, a convex sum of 2 vector points must lie on the line segment that joins the 2 points. A convex sum of 3 vector points must lie on the surface or the interior of the triangle joining the 3 vector points. A convex sum of 4 points could lie either on the surface or inside of a 3-dimensional polyhedron, or a 2-dimensional polygon (see figure 1.1).

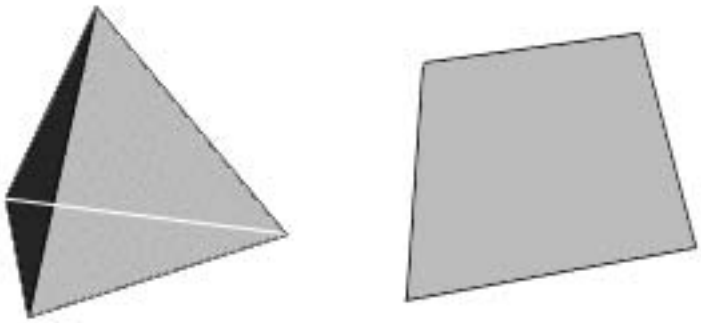

Figure 1.1: A convex sum of 4 points can either be 3D or 2D

A particular convex decomposition of a density matrix is of interest to us, and that is the canonical or eigen decomposition. Since a density matrix is hermitian, it can be diagonalized:

$$\rho = \sum_i \rho_i |\phi_i\rangle\langle\phi_i| \tag{1.4}$$

Each eigenvector appears as a pure state density matrix $|\phi_i\rangle\langle\phi_i|$, and the normalization condition (equation 1.3) requires $\sum_i \rho_i = 1$. Therefore the eigen decomposition is also a convex decomposition.

Notice that the pure state density matrices $|\phi_i\rangle\langle\phi_i|$ cannot be written as a convex sum of other states, therefore they must be extremal states of the convex set. For a convex set, extremal points are points on the convex hull. The convex hull is the set of points that generate the convex set. For example the convex hull of a triangle is the set of 3 vertices. Any point inside the convex set can be decomposed as a convex sum of the points on the hull. We note that the hull is not the same as the surface of the convex set, although the points in the hull do lie on the surface.

Every pure state is extremal so it must be an element of the convex hull.

Conversely, every density matrix can be decomposed as a convex sum of pure states by an eigen decomposition, so pure states can generate the convex set of density matrices. Therefore pure states form the convex hull for the set of density matrices.

There are some special features and symmetries of the convex set of density matrices that we can deduce from the eigen decomposition. In general, for a convex set of dimension D, any point on the interior of the set can be decomposed in terms of $D+1$ points on the hull. The set of $N \times N$ density matrices has dimension N^2-1, by this general rule for convex sets, it would require N^2 pure states for a convex decomposition. However, the eigen decomposition requires only $\leq N$ states. This demonstrates a symmetry in the convex set of density matrices.

The eigen decomposition uses the minimum number of extremal points in the decomposition; it is not possible to convexly decompose a density matrix with fewer extremal points. We can easily see that it is minimal since pure state matrices are rank 1 matrices, and we cannot decompose a rank M density matrix with less than M rank 1 matrices. This decomposition is also unique because we cannot decompose the density matrix in terms of any other set of M pure states unless there is a degeneracy in its eigenvalues.

This existence of a unique minimal decomposition is not a general feature of convex sets. Take for example a 2 dimensional convex figure (see figure 1.2) with 4 points (vertices) on the hull. Any point inside this set can be convexly decomposed in terms of a minimum of 3 points on the hull, however there are 2 minimum decompositions possible for most points inside the set.

We also observe a certain symmetry with the eigen decomposition itself. An eigen decomposition consists of N extremal points, but its coefficients must sum to 1, so it has only $N-1$ free coefficients. Therefore the eigen decomposition is

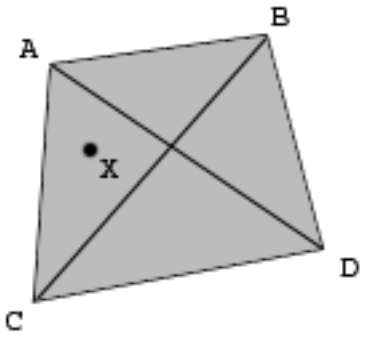

Figure 1.2: Point X can be convexly decomposed either by (A,B,C) or (A,D,C)

described by a $N-1$ dimensional convex figure with N vertices.

Now if we interchange the eigen states, we still get a valid density matrix. So this convex figure has to map to itself under interchange of the vertices. Such a convex figure is said to be regular.

A regular figure of N vertices in $N-1$ dimensions is known as a simplex or hypertetrahedron, and is labeled as Δ_{N-1}. A simplex is the simplest polytope possible for a given dimension. For example, the 1-dimensional simplex Δ_1 is a line segment, the 2-dimensional simplex Δ_2 is the equilateral triangle (see figure 1.3) and the 3-dimensional Δ_3 is the tetrahedron (see figure 1.4).

For clarity, we will call the simplex formed by a set of basis states a basis simplex.

If we take the set of density matrices, and regard all bases as equivalent, then the equivalence class is represented by a basis simplex. In other words, the set of density matrices modulo $SU(N)$ is just a simplex Δ_{N-1}. Conversely, we can think of the set of density matrices as being generated by the group $SU(N)$ acting on one basis simplex.

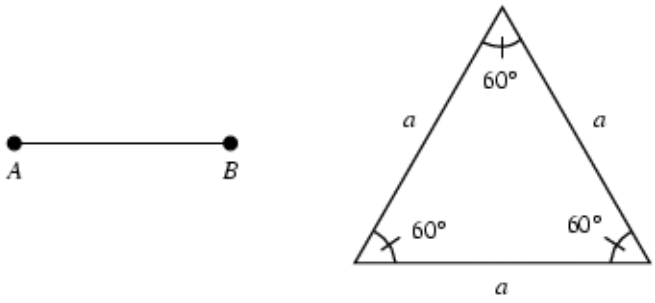

Figure 1.3: Line segment and equilateral triangle are the 1-dimension and 2-dimensional simplex respectively

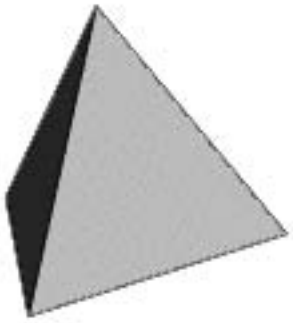

Figure 1.4: Tetrahedron is the 3-dimensional simplex

So we can see that the set of density matrices contains several symmetries, given by $SU(N)$ and the simplex Δ_{N-1}. It has features of both: the manifold has sharp edges and vertices as given by the simplex, but it also has continuous smooth surfaces given by $SU(N)$.

Let us consider the set of density matrices as a collection of infinitely many basis simplexes (as generated by $SU(N)$). We might want to know if any two basis simplexes overlap. For example, if we were to take a triangle that is centered about the origin, and rotate it about the origin, the original triangle and the rotated

triangle will have a non-zero overlap in general. For density matrices, we find that no two basis simplexes can overlap except along certain hyper planes of dimensions $N-2$ and less. Recall that the eigen decomposition is a unique minimal decomposition, so if two basis simplexes have an overlap, then a state that lies inside this overlap can be minimally decomposed in more than one way, which contradicts our statement about uniqueness. The only way this could happen is when two or more eigen values are degenerate. Therefore two basis simplexes can overlap along those points, lines and (hyper) planes where two or more eigen values are degenerate.

In fact there is a common intersection point for all basis simplexes, and that is at the center of the simplex. The center is the state with fully degenerate convex coefficients or eigenvalues. This matrix is often called the maximally mixed state, or randomly mixed state.

Now let us apply what we have learned to density matrices of a 2 state system. We know from other work that the convex set of 2×2 density matrices is given by a solid sphere, which is called the Bloch sphere. We can derive this independently from simple geometric considerations. Since $N = 2$, any density matrix has an eigen decomposition that is represented by the 2-dimensional simplex, which is a line segment. The eigen states are the extremal end points of the line segment.

The set of density matrices is then generated by $SU(2)$ on this line segment. Coincidentally $SU(2)$ modulo S_2 is $SO(3)$. So in this case it is not too difficult to visualize the set of density matrices being generated by the $SO(3)$ rotations acting on a line segment, which would give a solid sphere (figure 1.5). The extremal points of the line segment now forms the surface of the sphere, so the surface is the set of pure states. The interior points of the sphere are the mixed states. At the center of the sphere is the maximally mixed state $\rho = \frac{1}{2}I$.

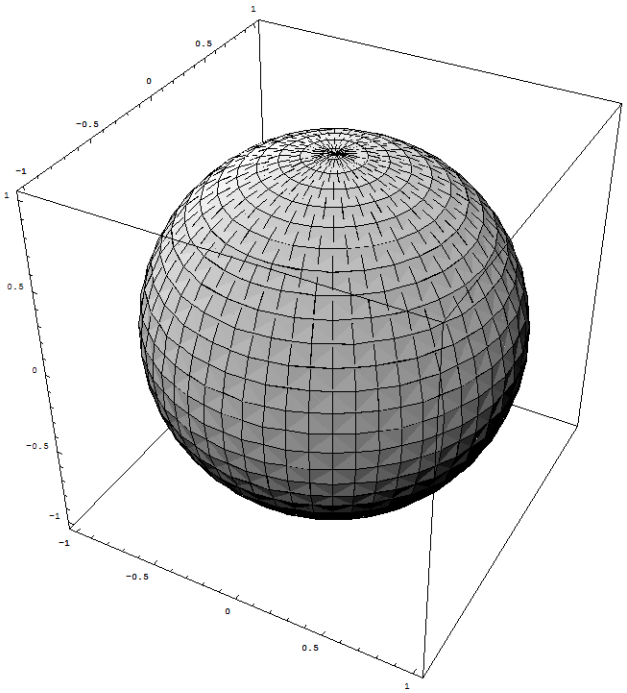

Figure 1.5: Bloch sphere: surface of pure states and interior of mixed states

Any point inside the sphere has a eigen decomposition that is given by drawing an axis passing through the point and the center of the sphere. Where the axis intersects the surface, we get 2 anti-podal points that are the pure eigen states of the density matrix. The line joining these two pure states is the unique basis simplex for all points that lie along that axis.

1.3 Density matrices as a real vector space

The space of $N \times N$ density matrices can also be represented by a $N^2 - 1$ real vector space, by writing the density matrix in the following fashion:

$$\rho = \frac{1}{N}(I + \overrightarrow{v} \cdot \overrightarrow{\sigma}) \tag{1.5}$$

where σ_i is a linearly independent (trace orthogonal) and complete set of traceless complex matrices. By writing the density matrix in this form the density matrix is automatically of unit trace. However there has to be constraints on $\overrightarrow{v}$ in order to keep ρ positive.

For $N = 2$, the natural choice for σ_i are the Pauli matrices. We can derive the condition for $\overrightarrow{v}$ such that ρ is positive. If we simply expand the matrix:

$$\rho = \frac{1}{2}\begin{pmatrix} 1+v_3 & v_1+iv_2 \\ v_1-iv_2 & 1-v_3 \end{pmatrix} \tag{1.6}$$

The necessary and sufficient conditions for the matrix to be positive are:

$$|v_3| \leq 1 \tag{1.7}$$

$$v_1^2 + v_2^2 + v_3^2 \leq 1 \tag{1.8}$$

So we find that the condition for ρ to be positive is simply given by $|\overrightarrow{v}|^2 \leq 1$. Interpreted geometrically, this is the equation for a solid sphere. So once again we arrive at the Bloch sphere for $N = 2$.

This treatment can in principle be extended to higher dimensions, however the conditions for positivity become much more complex.

We note that in this space, the convex sum of two density matrices is also the convex sum of the vectors:

$$\sum_i p_i \rho_i = \frac{1}{N}\left(I + (\sum_i p_i \overrightarrow{v_i}) \cdot \overrightarrow{\sigma}\right) \tag{1.9}$$

Therefore the convex structure of density matrices is retained.

1.4 Purification leads to a manifold for density matrices

We described in the first section how mixed states come about from statistical ensembles. But mixed states are perhaps more commonly the result of an open system, where the system in question is actually one part of a larger system. Take for example a large system comprising of many smaller systems labeled $\mathbb{A}, \mathbb{B}, \ldots$, where the overall system is in a pure state:

$$|\Psi\rangle = \sum_{ij\ldots} \alpha_{ij\ldots} |\psi_i^{\mathbb{A}}\rangle \otimes |\psi_j^{\mathbb{B}}\rangle \otimes |\ldots\rangle \tag{1.10}$$

Unless the overall system is in a product pure state, where $\alpha_{ij\ldots} \sim \delta_{ij\ldots}$, any sub-system we consider will be in a mixed state. The first sub-system $\mathbb{A}$ in this case would be given by partially tracing over all the other sub-systems. A partial trace is a trace performed only on a sub-system, so for example a partial trace over the $\mathbb{B}$ sub-system of a $\mathbb{AB}$ system is given by:

$$Tr_B \rho^{\mathbb{AB}} = \sum_i \langle i^{\mathbb{B}} | \rho^{\mathbb{AB}} | i^{\mathbb{B}} \rangle \tag{1.11}$$

where $|i^{\mathbb{B}}\rangle$ is a complete basis spanning the $\mathbb{B}$ system states. The partial trace gives us the density matrix of the $\mathbb{A}$ system, which correctly provides us all the expectation values of measurements if we were only allowed to measure the $\mathbb{A}$ system.

Returning to our original example, the partial trace of the large system gives:

$$\rho^{\mathbb{A}} = \sum_i \left(\sum_{j\ldots} \alpha_{ij\ldots}^2 \right) |\psi_i^{\mathbb{A}}\rangle \langle \psi_i^{\mathbb{A}}| \tag{1.12}$$

This is a mixed state unless the large system is in a product pure state. So mixed states are often the result of open systems. For instance this often occurs when

the particle is not perfectly isolated from the environment. The particle may have been initially prepared in a pure state, but through interaction with the environment, given by a unitary transformation of the system comprising the particle and the environment, the total system evolves into a non-product pure state. As a result the particle state becomes mixed. This effect is known as quantum decoherence.

Suppose we find that a system is in a mixed state. We may wonder if it is part of a larger system that is in a pure non-product state. This is the basic question of purification [35, 36]. Given a system that is in a mixed state, what pure state could the larger system be in?

Consider the canonical decomposition of a $N \times N$ mixed state:

$$\rho = \sum_{i}^{N} \rho_i |\psi_i\rangle\langle\psi_i| \tag{1.13}$$

We can write a pure state in N^2 dimension that would be a purification of the mixed state above:

$$|\Psi\rangle = \sum_{i}^{N} \sqrt{\rho_i} |\psi_i\rangle |i^{\mathbb{B}}\rangle \tag{1.14}$$

where $|i^{\mathbb{B}}\rangle$ forms an orthornormal set of states. We can check that the partial trace of this pure state gives us the mixed state we started with:

$$Tr_{\mathbb{B}}[|\Psi\rangle\langle\Psi|] = \rho \tag{1.15}$$

From this relatively simple procedure we see that mixed states can always be given as a partial trace of a pure state. Mathematically, we cannot distinguish whether a mixed state is a result of an open system or if it was prepared as a statistical ensemble.

We are interested in purification because pure states are well understood, while the set of mixed states is not as well understood in many ways. We know the set of pure states form a manifold CP^N, the complex projective space of rays (since pure states vectors are normalized) in the complex vector space of N dimensions C^N. CP^N is a well understood manifold, it is compact and simply connected, and carries the Fubini-Study metric. Since we study pure states as vectors that are normalized, CP^N is probably best visualized as $2N+1$ sphere modulo $U(1)$ to eliminate the vector length (to get rays), $S^{2N+1}/U(1)$.

On the other hand we have density matrices – we know density matrices are complex positive hermitian matrices of unit trace, but we do not know the manifold and structure of these states. Our objective here is to derive the manifold and structure from CP^N given that purification gives us an association between density matrices and pure states.

Looking back at the purification procedure, we see that it is always possible to find a purification for a density matrix, but the purification is not unique; several pure states can have the same partial trace. Therefore purification is an injection (one to many), and conversely partial trace is a surjection (many to one).

With purification, $N \times N$ density matrices are mapped to N^2 dimensional pure states. So we can start with the manifold of N^2 dimensional pure states which is CP^{N^2-1}, and to get from pure states to $N \times N$ density matrices we take the partial trace. Partial trace is a surjective functional, so we need to identify the orbit of pure states that correspond to each density matrix.

We can show that these orbits are given by $I \otimes SU(N)$. First we prove that 2 pure states in a N^2 dimensional Hilbert space $|\Psi\rangle$ and $|\Phi\rangle$, with the same partial trace:

$$Tr_{\mathbb{B}}[|\Psi\rangle\langle\Psi|] = Tr_{\mathbb{B}}[|\Phi\rangle\langle\Phi|] \tag{1.16}$$

are connected by a unitary transformation $V \in SU(N)$, such that $I \otimes V|\Psi\rangle = |\Phi\rangle$.

To begin this proof, let us first write the 2 states in their Schmidt decomposition:

$$|\Psi\rangle = \sum_{k}^{\mu} \alpha_k |\psi_k^{\mathbb{A}}\rangle|\psi_k^{\mathbb{B}}\rangle \tag{1.17}$$

$$|\Phi\rangle = \sum_{q}^{\nu} \beta_q |\phi_q^{\mathbb{A}}\rangle|\phi_q^{\mathbb{B}}\rangle \tag{1.18}$$

If their partial traces are equal, then:

$$\sum_{k}^{\mu} \alpha_k^2 |\psi_k^{\mathbb{A}}\rangle\langle\psi_k^{\mathbb{A}}| = \sum_{q}^{\nu} \beta_q^2 |\phi_q^{\mathbb{A}}\rangle\langle\phi_q^{\mathbb{A}}| \tag{1.19}$$

For the equality to hold, we can see several conditions have be met:

$$\mu = \nu \tag{1.20}$$

$$\alpha_k^2 = \beta_k^2 \quad \text{for suitably ordered values} \tag{1.21}$$

If no values α_k^2 are degenerate then we can simply equate the basis states (upto an arbitrary phase):

$$|\psi_k^{\mathbb{A}}\rangle = e^{i\xi_k}|\phi_k^{\mathbb{A}}\rangle \tag{1.22}$$

Therefore in the non-degenerate case, the only freedom we have is in speci-

fying the $\mathbb{B}$ bases: $\{|\psi_k^{\mathbb{B}}\rangle\}$ and $\{|\phi_q^{\mathbb{B}}\rangle\}$. The difference between the 2 bases is given by a unitary transformation in the $\mathbb{B}$ system.

If a degeneracy exists, the problem is a little more complicated. If the eigenvalues that are degenerate are given by α_z^2, for particular values of z, then the states $|\psi_z^{\mathbb{A}}\rangle$ and $|\phi_z^{\mathbb{A}}\rangle$ can differ by an unitary transform. But we can show that this unitary transformation can be equivalently performed in the $\mathbb{B}$ system. Consider the terms in $|\Psi\rangle$ for which the Schmidt coefficients are degenerate:

$$\sum_z C|\psi_z^{\mathbb{A}}\rangle|\psi_z^{\mathbb{B}}\rangle \tag{1.23}$$

If we perform a unitary transformation V within the sub-space spanned by $|\psi_z^{\mathbb{A}}\rangle$, that would give:

$$\begin{aligned} V \otimes I \sum_z C|\psi_z^{\mathbb{A}}\rangle|\psi_z^{\mathbb{B}}\rangle &= \sum_{zz'} CV_{zz'}|\psi_{z'}^{\mathbb{A}}\rangle|\psi_z^{\mathbb{B}}\rangle \\ &= \sum_{zz'} C|\psi_z^{\mathbb{A}}\rangle V_{z'z}|\psi_{z'}^{\mathbb{B}}\rangle \\ &= I \otimes V^T \sum_z C|\psi_z^{\mathbb{A}}\rangle|\psi_z^{\mathbb{B}}\rangle \end{aligned} \tag{1.24}$$

So we see that when the coefficients are degenerate, $V \otimes I|\Psi\rangle = I \otimes V^T|\Psi\rangle$. Again the connection between $|\Psi\rangle$ and $|\Phi\rangle$ is a unitary transformation in the $\mathbb{B}$ system.

And finally, we know from equation 1.21 that the Schmidt coefficients of $|\Psi\rangle$ and $|\Phi\rangle$ have to be equal in magnitude, but they can differ by a (complex) phase. A unitary transformation in the $\mathbb{B}$ system can be used to alter the phase of the Schmidt coefficients. We note that an overall phase is irrelevant, so the group we are interested in is still $SU(N)$ and not $U(N)$. This concludes our proof that two pure states with the same partial trace are connected by a unitary transformation of the $\mathbb{B}$ system.

With this result we can see now that each $N \times N$ density matrix corresponds to a $I \otimes SU(N)$ orbit on CP^{N^2-1}. These orbits do not overlap, since $I \otimes SU(N)$ is a closed group. If 2 different orbits have a common intersection, then there exists a unitary transformation $I \otimes U$ from one orbit to the other, implying that the 2 orbits are identical, which is a contradiction.

Using purification, we have derived a bijective mapping between the manifold $CP^{N^2-1}/SU(N)$ and the set of density matrices. This mapping is invertible and smooth, so we can state that the manifold of density matrices is diffeomorphic to $CP^{N^2-1}/SU(N)$. Unfortunately the mapping is not a homomorphism, because additive properties are not preserved – we can confirm that the convex sum of two density matrices is not the same as the partial trace of the convex sum of the two purified states.

1.5 Schmidt strata

Although the manifold $CP^{N^2-1}/SU(N)$ is not strictly homormorphic to the set of density matrices, there are some interesting properties of this manifold that gives us extra insight into the geometry of density matrices.

In this section we will show that the manifold $CP^{N^2-1}/SU(N)$ is stratified. A stratified manifold is composed of disjoint subsets called strata. As we will see the strata have different dimensions and are classified according to Schmidt number, which is the number of non-zero coefficients of the Schmidt decomposition of the pure state.

The stratification of the manifold comes about because the $SU(N)$ orbits on CP^{N^2-1} are not all the same size. Let us consider the action of $I \otimes SU(N)$ on a pure state from the manifold CP^{N^2-1}:

$$I \otimes U \sum_{k}^{\mu} \alpha_k |\psi_k^{\mathbb{A}}\rangle |\psi_k^{\mathbb{B}}\rangle \tag{1.25}$$

where μ is the Schmidt number of the state. If $\mu < N$ then this action is not free – there could exist another unitary transformation W for which $I \otimes U|\Psi\rangle = I \otimes W|\Psi\rangle$. For a state with Schmidt number μ, the orthornormal states $|\psi_k^{\mathbb{B}}\rangle$ would span a μ dimensional subspace, any transformation performed outside of (orthogonal to) this subspace will not change the state. So the stabilizer of this action is $U(N-\mu)$.

Remember the rank of the density matrix is the same as the Schmidt number of the purification:

$$Tr_{\mathbb{B}}[|\Psi\rangle\langle\Psi|] = \rho = \sum_{k}^{\mu} \alpha_k^2 |\psi_k^{\mathbb{A}}\rangle\langle\psi_k^{\mathbb{A}}| \tag{1.26}$$

Therefore the orbit on CP^{N^2-1} corresponding to a density matrix with rank μ is accurately given by $I \otimes SU(N)/U(N-\mu)$.

The different strata are due to the different stabilizer groups, and because the groups are of different dimension, the strata would also be of different dimension. The dimension of CP^{N^2-1} is $2N^2-2$ and the dimension of $SU(N)$ is N^2-1. This gives us the expected dimension of N^2-1 for $N \times N$ density matrices. For states with maximal Schmidt number $\mu = N$, the stabilizer is the trivial group 1, the dimension of that stratum is N^2-1. As the Schmidt number decreases, the stabilizer group increases, and the dimension of the stratum decreases. For rank μ matrices, the stratum is $\mu(2N-\mu)-1$ dimensional. The lowest dimensional stratum is $2N-2$, which is the set of pure states, ie. the manifold CP^{N-1}.

Therefore the set of density matrices is a union of strata of dimensions given by $\mu(2N-\mu)-1$, with $1 \geq \mu \geq N$. The lowest dimensional stratum, a $2N-2$

dimensional surface, forms the set of pure states.

Let us reconcile this with what we know about the convex nature of density matrices. We know a rank μ density matrix can always be decomposed in terms of rank $\mu - 1$ density matrices. That means a lower dimensional strata is a convex convering for higher dimensional strata. The lowest dimensional stratum, of the set of pure states, we already know is the convex hull for all density matrices.

Putting everything together, we can visualize the strata like the layers of an onion, the lower dimensional strata wrapped around the higher dimensional strata, the outermost layer being pure states and the innermost layer are the full rank density matrices. However, with an onion the layers are all the same dimension, so perhaps a more accurate analogy is a polytope. Take a simple 3 dimensional polytope, a pyramid. The 2 dimensional triangular faces are a convex covering for the interior of the pyramid, and the 1 dimensional edges are in turn a convex covering for the faces.

In fact, we remember something very similar from the eigen decomposition of density matrices. Any density matrix can be placed inside a $N-1$ dimension simplex Δ_{N-1}, the very interior of the simplex is occupied by density matrices of full rank N. The vertices of the simplex are the pure states (rank 1 density matrices), the edges are rank 2 density matrices, and the μ dimensional face are rank $\mu+1$ density matrices. We can understand the similarity, since we know that the set of density matrices is generated by $SU(N)$ on a basis simplex. The different dimensional faces of the simplex taken through $SU(N)$ give the different dimensional strata.

1.6 Distance measure for the manifold

In quantum mechanics there is a natural measure of distance between 2 pure states:

$$cos^2 d(\Phi, \Psi) = |\langle \Phi | \Psi \rangle|^2 \tag{1.27}$$

This distance has a maximum of $\pi/2$. In comparison, the Fubini-Study distance for the manifold CP^N is:

$$d_{Fubini-Study}(\Phi, \Psi) = \sqrt{2 - 2|\langle \Phi | \Psi \rangle|} \tag{1.28}$$

These two distances are compatible, the quantum mechanical distance is actually a round metric (angle) version of the Fubini-Study distance. So for pure states, both the mathematics of the manifold and quantum mechanics agree on a distance between 2 pure states.

Unfortunately there is no clear consensus on a distance measure for density matrices. Perhaps the most well known distance measure for density matrices is the Hilbert-Schmidt distance, which is often used in quantum optics:

$$d_{HS}(\rho, \tau) = \sqrt{Tr[(\rho - \tau)^2]} \tag{1.29}$$

Alternatively a slightly different distance measure is the trace distance [37, 38]:

$$d_{tr}(\rho, \tau) = Tr[\sqrt{(\rho - \tau)^2}] \tag{1.30}$$

Another approach is to derive a distance measure from the manifold $CP^{N^2-1}/SU(N)$. If this manifold represents density matrices, then there is a natural metric for this manifold inherited through the Fubini-Study metric of the parent manifold CP^{N^2-1}. Very simply, the distance between two orbits, representing two different density matrices, on CP^{N^2-1}, is the minimum Fubini-Study distance be-

tween any two points on two different orbits.

So let us consider two density matrices ρ and τ, and write them in their diagonal form:

$$\rho = \sum_i \alpha_i^2 |\psi_i\rangle\langle\psi_i| \tag{1.31}$$

$$\tau = \sum_i \beta_i^2 |\phi_i\rangle\langle\phi_i| \tag{1.32}$$

Let the pure states $|\Psi\rangle$ and $|\Phi\rangle$ be purifications of ρ and τ respectively:

$$|\Psi\rangle = \sum_i \alpha_i |\psi_i\rangle |i^{\mathbb{B}}\rangle \tag{1.33}$$

$$|\Phi\rangle = \sum_i \beta_i |\phi_i\rangle |i^{\mathbb{B}}\rangle \tag{1.34}$$

The Fubini-Study distance between $|\Psi\rangle$ and $|\Phi\rangle$ is:

$$d_{Fubini-Study}(\Psi, \Phi) = \sqrt{2 - 2|\langle\Psi|\Phi\rangle|} \tag{1.35}$$

Let us define P and T as follows:

$$P|\psi_i\rangle \rightarrow |i^{\mathbb{B}}\rangle \tag{1.36}$$

$$T|\phi_i\rangle \rightarrow |i^{\mathbb{B}}\rangle \tag{1.37}$$

This allows us to write:

$$P\rho^{1/2} = \alpha_i |i^{\mathbb{B}}\rangle\langle\psi_i| \tag{1.38}$$

$$\tau^{1/2}T^{\dagger} = \beta_i |\phi_i\rangle\langle i^{\mathbb{B}}| \tag{1.39}$$

The inner product $\langle\Psi|\Phi\rangle$ can then be expressed as:

$$\langle\Psi|\Phi\rangle = Tr_{\mathbb{B}}[P\rho^{1/2}\tau^{1/2}T^{\dagger}] \tag{1.40}$$

The states $|\Psi\rangle$ and $|\Phi\rangle$ are a particular purification of the density matrices ρ and τ. Of course we know that many other purifications exist, the orbits can be generated from one purification by $I \otimes SU(N)$. Our objective is to find the shortest distance between the two orbits that give ρ and τ. The minimum distance between two orbits is obtained by finding the maximum value for:

$$\max_{U,V}(I \otimes U|\Psi\rangle)^{\dagger}(I \otimes V|\Phi\rangle) \tag{1.41}$$

We can re-write this as:

$$\max_{U,V} Tr[UP\rho^{1/2}\tau^{1/2}T^{\dagger}V^{\dagger}] \tag{1.42}$$

Let us define:

$$M = UP\rho^{1/2}\tau^{1/2}T^{\dagger}V^{\dagger} \tag{1.43}$$

Now to find the maximum trace for M, let us take the singular value decomposition of M:

$$M = WDX \tag{1.44}$$

where W and X are unitary transformations, and D is a diagonal matrix with the singular values of M. This will allow us to write the trace of M as:

$$Tr[M] = \sum_{ij} W_{ji} D_i X_{ij} = \sum_i Z_{ii} D_i \tag{1.45}$$

where $Z = XW$.

Since D is diagonal, the only elements of Z needed to compute the trace are the diagonal elements. Z is also unitary, so its diagonal elements are of the form:

$$Z_{ii} \sim cos(\theta_i) \leq 1 \tag{1.46}$$

The trace of M is therefore maximized when all the elements $Z_{ii} = 1$, which implies $Z = I$.

We can now write the distance between two density matrices ρ and τ as:

$$d(\rho, \tau) = \sqrt{2 - 2Tr[D]} \tag{1.47}$$

This is the minimum Fubini-Study distance between 2 pure states, one on the orbit of purified states of ρ and the other on the orbit of purified states of τ.

We can further express this distance in terms of the density matrices ρ and τ. We can work backwards from D. We know $M = WDX \Rightarrow D = W^\dagger M X^\dagger$, now consider D^2:

$$D^2 = (W^\dagger M X^\dagger)(W^\dagger M X^\dagger)^\dagger = W^\dagger M^2 W \tag{1.48}$$

Substituting the original form for M, we get:

$$\begin{aligned} D^2 &= W^\dagger M^2 W \\ &= W^\dagger (UP\rho^{1/2}\tau^{1/2}T^\dagger V^\dagger)(UP\rho^{1/2}\tau^{1/2}T^\dagger V^\dagger)^\dagger W \\ &= W^\dagger UP\rho^{1/2}\tau\rho^{1/2}P^\dagger U^\dagger W \end{aligned} \tag{1.49}$$

We can therefore write D as:

$$D = Z(\rho^{1/2}\tau\rho^{1/2})^{1/2}Z^\dagger \tag{1.50}$$

where $Z = W^\dagger UP$ is a unitary transformation. Finally we can write:

$$d(\rho,\tau) = \sqrt{2 - 2Tr[(\rho^{1/2}\tau\rho^{1/2})^{1/2}]} \tag{1.51}$$

This distance is called the Bures distance for density matrices [39, 40, 41]. We could also use the round metric instead to obtain an angular separation between density matrices, this distance is given by:

$$d_{round}(\rho,\tau) = \sqrt{2sin^{-1}(1 - Tr[(\rho^{1/2}\tau\rho^{1/2})^{1/2}])} \tag{1.52}$$

Chapter 2

Generalized linear quantum operations

We will begin by reviewing dynamical maps, their canonical decomposition and connection to unitary transformations [15, 16]. We will also review extremal maps [24] and dynamical maps as affine geometrical transformations [22].

This purpose of this chapter is to lay the foundation for later discussions, however we do provide a new calculation for the volume of dynamical maps.

2.1 Dynamical maps

In basic quantum mechanics, the operations on quantum states are unitary transformations. When dealing with density matrices, the operations can be more complex.

Any linear transformation or map of a $N \times N$ density matrix can be given by a super-matrix of $N^2 \times N^2$ dimension, which we can write as follows:

$$\rho_{rs} \to \mathcal{A}_{rs,r's'}\rho_{r',s'} \tag{2.1}$$

We will call this representation of the map the A-matrix. The A-matrix is of limited usefulness to us, but with a simple re-arrangement of the indices, we can get an alternative representation:

$$\rho_{rs} \rightarrow \mathcal{B}_{rr',ss'}\rho_{r',s'} \tag{2.2}$$

We will call this representation the B-matrix [15]. The B-matrix is useful because it is hermitian. This comes from requiring that the map transform hermitian density matrices to hermitian density matrices:

$$\begin{aligned} \rho'_{r,s} &= \mathcal{B}_{rr',ss'}\rho_{r',s'} \\ &= \mathcal{B}^*_{ss',rr'}\rho^*_{s',r'} \\ &= {\rho'_{s,r}}^* \end{aligned} \tag{2.3}$$

In addition to preserving hermiticity, for the map to be physical it should also preserve the trace and positivity of the density matrix. To preserve trace, the map has to satisfy:

$$Tr[\rho'] = Tr[\rho] \Rightarrow \sum_r \mathcal{B}_{rr',rs'} = \delta_{r',s'} \tag{2.4}$$

To preserve positivity the B-matrix should be positive:

$$\mathcal{B} \geq 0 \tag{2.5}$$

We note that this condition is known as complete positivity. A physical map does not always have to be completely positive, however it can only work on a restricted domain of states (ie. not all density matrices). This issue is a little complicated, we will leave the discussion to later chapters, and for now we will work

with the assumption of complete positivity.

We also note that in certain situations we may be interested in maps that can reduce the trace of density matrices. This can be interpreted as a loss of the particle from the apparatus, or that the map acts as a sort of measurement projection. We will elaborate on these maps in the next chapter. We should note that maps that increase the trace of density matrices can have no physical interpretation, so they will not considered.

So we will deal with maps that are completely positive and trace preserving, which we will call dynamical maps. Dynamical maps form a closed convex set. Consider a convex sum of dynamical maps:

$$\mathcal{D} = \sum_i p_i \mathcal{B}^{(i)} \quad ; \sum_i p_i = 1 \tag{2.6}$$

$\mathcal{D}$ preserves hermiticity:

$$\begin{aligned} \mathcal{D}_{rr',ss'}\rho_{r',s'} &= \textstyle\sum_i p_i [\mathcal{B}^{(i)}]_{rr',ss'}\rho_{r',s'} \\ &= \textstyle\sum_i p_i [\mathcal{B}^{(i)}]^*_{ss',rr'}\rho^*_{s',r'} \\ &= \mathcal{D}^*_{ss',rr'}\rho^*_{s',r'} \end{aligned} \tag{2.7}$$

$\mathcal{D}$ preserves positivity since:

$$\mathcal{D}(\rho) = \sum_i p_i \mathcal{B}^{(i)}(\rho) \quad p_i \geq 0, \mathcal{B}^{(i)}(\rho) \geq 0 \Rightarrow \mathcal{D}(\rho) \geq 0 \tag{2.8}$$

Finally $\mathcal{D}$ preserves trace since:

$$Tr[\mathcal{D}(\rho)] = \sum_i p_i Tr[\mathcal{B}^{(i)}(\rho)] = \sum_i p_i Tr[\rho] = Tr[\rho] \tag{2.9}$$

Therefore a convex sum of dynamical maps is also a dynamical map.

2.2 Dynamical maps decomposition

Since the B-matrix is a hermitian matrix, it can be diagonalized [14, 15, 16]. The B-matrix is a $N^2 \times N^2$ matrix, so its canonical decomposition would consist of $\nu \leq N^2$ eigen-vectors with real eigenvalues:

$$\mathcal{B}_{rr',ss'} = \sum_{\alpha}^{\nu} c_\alpha [C_\alpha]_{rr'} [C_\alpha]^*_{ss'} \tag{2.10}$$

When the map acts on a density matrix, we notice that the eigen-vectors C_α act as bi-linear operators on the density matrix:

$$[\mathcal{B}(\rho)]_{rs} = \sum_{\alpha r's'} c_\alpha [C_\alpha]_{rr'} \rho_{r's'} [C_\alpha]^\dagger_{s's} \tag{2.11}$$

The condition that the map preserves the trace of the density matrix becomes:

$$\sum_{\alpha r} c_\alpha [C_\alpha]^\dagger_{s'r} [C_\alpha]_{rr'} = \delta_{r's'} \tag{2.12}$$

and the condition that the map is completely positive requires all eigen-values $c_\alpha \geq 0$.

For clarity in later discussions, we will call the eigen-values of a map as c-values and the eigen-matrices of the map as C-matrices. We note that C-matrices are often referred to as Kraus operators [23], although these matrices were first given more than two decades earlier in [15].

We also note that in most papers the C-matrices are usually normalized by $C_\alpha \to \sqrt{c_\alpha} C_\alpha$ so as to set the c-values to 1. However in this thesis we will normalize the C-matrices with the trace orthonormality condition $Tr[C_\alpha C^\dagger_\beta] = \delta_{\alpha\beta}$, as this

property will be useful in some discussions.

2.3 Dynamical maps and unitary transformations

In the last chapter we discussed purification, where any density matrix can be written as a reduced form (through partial trace) of a pure state. In a similar fashion, dynamical maps can be written as a reduced form of a unitary transformation in a larger system [24].

Let us consider a unitary transformation U acting on a larger system, which consists of the original system $\mathbb{A}$ coupled with an ancillary system $\mathbb{B}$ of ν dimensions. Let system $\mathbb{A}$ be spanned by a basis $|r\rangle$ and system $\mathbb{B}$ be spanned by a basis $|\alpha\rangle$. The $\mathbb{AB}$ system is spanned by a basis:

$$|r\rangle|\alpha\rangle \quad ; 0 \geq r \geq N-1, 0 \geq \alpha \geq \nu - 1 \tag{2.13}$$

Let us define a transformation U, given by:

$$U : |r'\rangle|0\rangle \rightarrow \sum_{r\alpha} \sqrt{c_\alpha}\, [C_\alpha]_{rr'}\, |r\rangle|\alpha\rangle \tag{2.14}$$

Our definition is incomplete, because we have not specified how U transforms a complete basis of states. Specifically, we have not defined how U transforms the states $|r'\rangle|\alpha\rangle$ for $\alpha \neq 0$. But given the transformation as defined, we may ask the question whether it is consistent with a unitary transformation. This can be accomplished by checking if U preserves the orthornormality between states $|r'\rangle|0\rangle$ and $|s'\rangle|0\rangle$:

$$(\langle s'|\langle 0|U^\dagger)(U|r'\rangle|0\rangle) = \sum_{r\alpha} c_\alpha [C_\alpha]^\dagger_{s'r} [C_\alpha]_{rr'} = \delta_{r',s'} \tag{2.15}$$

The last equality is satisfied by the condition that the map preserves trace, as given by equation 2.12. So we can confirm that U does in fact preserve orthornormality between the states it is defined on. We can then "complete" the transformation U by defining transformations for states $|r'\rangle|\alpha\rangle$ where $\alpha \neq 0$, making sure to transform them into a space orthogonal to the space spanned by $U|r'\rangle|0\rangle$. We need not concern ourselves with how U is completed, in fact it can be completed in many ways so there is no one unique transformation, but our main concern is that a unitary transformation U exists.

Now if we take our original density matrix ρ and couple it to an ancillary system $\mathbb{B}$ initially in the state $|0\rangle\langle 0|$, and apply the unitary transformation U, that will give us:

$$\sum_{rr'ss'\alpha\beta} \sqrt{c_\alpha}\sqrt{c_\beta}[C_\alpha]_{rr'}\rho_{r's'}[C_\beta]^\dagger_{s's}|r\alpha\rangle\langle s\beta| \tag{2.16}$$

If we trace over the ancillary system $\mathbb{B}$, that will gives:

$$\rho'_{rs} = \sum_{r's'\alpha} c_\alpha[C_\alpha]_{rr'}\rho_{r's'}[C_\alpha]^\dagger_{s's} = [\mathcal{B}(\rho)]_{rs} \tag{2.17}$$

This gets us back to the desired map $\mathcal{B}(\rho)$. Therefore any trace-preserving map can be thought of as the contraction of a unitary transformation acting on a larger system, by suitably coupling a reservoir of dimension $\nu \leq N^2$ to the original system. More specifically, we can write:

$$\mathcal{B}(\rho) = Tr_{\mathbb{B}}[U\mathcal{E}(\rho)U^\dagger] \tag{2.18}$$

where $\mathcal{E}$ is what we call an extension map [42], which is defined here as:

$$\mathcal{E}(\rho) = \rho \otimes |0\rangle\langle 0| \tag{2.19}$$

2.4 Volume of the set of dynamical maps

The last section gave us a relationship between the set of maps on $N \times N$ density matrices and the set of unitary transformations on a N^3 dimensional (N dimensions of the original system plus upto N^2 dimension for the auxillary system) Hilbert space, $SU(N^3)$.

Much like what we did with density matrices, we want to find the orbits of $SU(N^3)$ that correspond to each map. Recall that we had left a great deal of freedom to complete the unitary transformation, and that the transformation we were interested in was not defined on a complete basis of states. In fact, the transformation we need was only defined on N basis states $|r'\rangle|0\rangle$ where $0 \leq r' \leq N-1$, out of a complete N^3 basis states.

We stated that it was unimportant how the transformation acts on the remaining $N^3 - N$ basis states $|r'\rangle|\alpha\rangle$ where $1 \leq \alpha \leq N^2 - 1$, other than requiring that it is consistent as a unitary transformation. This freedom can be expressed as a equivalence relationship – for any $V \in SU(N^3 - N)$, the following maps are equivalent:

$$\mathcal{B}(\rho) = Tr_{\mathbb{B}}[U\mathcal{E}(\rho)U^\dagger] = Tr_{\mathbb{B}}[UV\mathcal{E}(\rho)V^\dagger U^\dagger] \tag{2.20}$$

Therefore we conclude that the set of maps is bijective with the coset space $SU(N^3)/SU(N^3 - N)$.

We can perform some straightforward calculations to obtain the volume of

the coset space $SU(N^3)/SU(N^3-N)$. The volume of $SU(M)$ has been given [31, 32] as:

$$V_{SU(M)} = 2^{\frac{M-1}{2}} \pi^{\frac{(M-1)(M+2)}{2}} M^{\frac{1}{2}} \prod_{k=1}^{M-1} \frac{1}{k!} \tag{2.21}$$

Therefore, the volume of $SU(N^3)/SU(N^3-N)$ is:

$$\begin{aligned} V_{\frac{SU(N^3)}{SU(N^3-N)}} &= 2^{\frac{N}{2}} \pi^{\frac{2N^4-N^2-3N}{2}} \frac{N}{\sqrt{N^2-1}} \prod_{k=N^3-N}^{N^3-1} \frac{1}{k!} \\ &= 2^{\frac{N}{2}} \pi^{N^4-N^2+1} \frac{N}{\sqrt{N^2-1}} \prod_{k=1}^{N} \frac{1}{(N^3-k)!} \end{aligned} \tag{2.22}$$

2.5 Extremal maps

Since dynamical maps form a closed convex set, there will be extremal points to the set. In the context of convex sets, a map is extremal if it cannot be convexly decomposed in terms of other maps.

With density matrices, we know that the extremal density matrices are the rank 1 density matrices, in other words the pure projections. With dynamical maps, the rank 1 maps are the unitary maps. We can see this from:

$$\mathcal{B}(\rho) = C\rho C^\dagger \tag{2.23}$$

The requirement that the map $\mathcal{B}$ preserve trace is:

$$C^\dagger C = I \tag{2.24}$$

Therefore C is simply a unitary matrix.

However the rank 1 maps are not the only extremal maps [24]. For a generic map $\mathcal{B}$ with C-matrices C_α, there is no constraint on the C-matrices that they have

to individually satisfy $C_\alpha^\dagger C_\alpha = I$, so each C-matrix need not be unitary in form. Perhaps not all maps can be convexly decomposed in terms of unitary maps, in which case there may be more extremal maps we need to consider.

The key to identifying the extremal maps is found in the condition for the maps to be trace preserving:

$$\sum_{r\alpha} c_\alpha [C_\alpha]^\dagger_{s'r} [C_\alpha]_{rr'} = \delta_{r's'} \tag{2.25}$$

Let us define:

$$[D_\alpha]_{r's'} = \sum_r [C_\alpha]^\dagger_{s'r} [C_\alpha]_{rr'} \tag{2.26}$$

We notice that D is hermitian:

$$[D_\alpha]_{r's'} = ([C_\alpha]_{rs'} [C_\alpha]^*_{rr'})^* = [D_\alpha]^*_{s'r'} \tag{2.27}$$

The trace preserving condition is now:

$$\sum_\alpha c_\alpha [D_\alpha]_{r's'} = \delta_{r's'} \tag{2.28}$$

On the RHS we have a rank N matrix. For the LHS, the D_α matrices are hermitian, and we know that having more than N hermitian matrices would be over-complete. Therefore if there are more than N terms on the LHS, then the D_α matrices cannot all be linearly independent. In that case there exists a relationship between the D_α:

$$\sum_\alpha k_\alpha D_\alpha = 0 \tag{2.29}$$

We can then define two maps $\mathcal{B}^+$ and $\mathcal{B}^-$ as follows:

$$\mathcal{B}^{\pm}(\rho) = \sum_{\alpha}(c_\alpha \pm \epsilon k_\alpha) C_\alpha \rho C_\alpha^\dagger \tag{2.30}$$

For sufficiently small ϵ, both maps are completely positive. Also both maps preserve trace since:

$$\left(\sum_{\alpha} c_\alpha D_\alpha\right) \pm \epsilon \left(\sum_{\beta} k_\beta D_\beta\right) = I \tag{2.31}$$

Now we can express our map $\mathcal{B}$ as:

$$\mathcal{B} = \frac{1}{2}\left(\mathcal{B}^+ + \mathcal{B}^-\right) \tag{2.32}$$

Therefore if the map $\mathcal{B}$ has more than N C-matrices, then it cannot be extremal since it can be expressed as a convex sum of two other maps.

Conversely, we can show that it is sufficient for a map to be extremal, if $C_\beta^\dagger C_\alpha$ are all linearly independent. If the map $\mathcal{B}$ is not extremal, then without any loss of generality we can decompose $\mathcal{B}$ as the midpoint of a cord between two other maps, such that $\mathcal{B} = 1/2(\mathcal{B}^+ + \mathcal{B}^-)$. In general, we can write $\mathcal{B}^{\pm}$ as:

$$\mathcal{B}^{\pm} = \mathcal{B} \pm \sum_{\alpha\beta} x_{\alpha\beta} C_\alpha \rho C_\beta^\dagger \tag{2.33}$$

This is a more general form than what was previously discussed since off-diagonal terms are included. The trace preservation condition gives:

$$\sum_{\alpha\beta} x_{\alpha\beta} C_\beta^\dagger C_\alpha = 0 \tag{2.34}$$

This can only be satisfied if the matrices $C_\beta^\dagger C_\alpha$ are not linearly dependent. Therefore if $C_\beta^\dagger C_\alpha$ are linearly independent, then we cannot convexly decompose the map $\mathcal{B}$ in terms of two other maps.

We conclude that a map is extremal if and only if it has $\leq N$ C-matrices such that $C_\beta^\dagger C_\alpha$ are linearly independent.

A pin map is the simplest example of such an extremal map. A pin map will map all density matrices to a fixed pure state:

$$\mathcal{B}(\rho) = |\Phi\rangle\langle\Phi| \tag{2.35}$$

The C-matrices of this map are given by:

$$C_i = |\Phi\rangle\langle i| \tag{2.36}$$

where the states $|i\rangle$ form a complete basis, so $0 \leq i \leq N-1$. Therefore the map is effectively:

$$\sum_i |\Phi\rangle\langle i|\rho|i\rangle\langle\Phi| \tag{2.37}$$

Now we can see how all density matrices will be mapped to the fixed pure state $|\Phi\rangle$. We contrast this to a unitary transformation, where instead of a fixed $|\Phi\rangle$, it would be an orthonormal set $|\Phi_i\rangle$:

$$\sum_i |\Phi_i\rangle\langle i|\rho|i\rangle\langle\Phi_i| \tag{2.38}$$

So the difference is that the unitary map takes an orthonormal basis to an orthonormal basis, while the rank N extremal map need not preserve orthogonality between the transformed basis states. It is clear that such extremal maps cannot

be composed in terms of unitary maps.

We also note that such extremal maps are in general not invertible. Clearly the pin map is not invertible, since all information in the density matrix is destroyed. Therefore the set of maps form a semi-group; a composition of dynamical maps is also a dynamical map:

$$\mathcal{D} \circ \mathcal{B}(\rho) = \mathcal{D}\left(\mathcal{B}(\rho)\right) \tag{2.39}$$

since it preserves hermiticity, trace and positivity. However not all maps have an inverse such that:

$$\mathcal{B}^{-1}\left(\mathcal{B}(\rho)\right) = \rho \tag{2.40}$$

2.6 Geometric mappings

Let us consider the representation of density matrices as vectors in a real vector space, where the vectors are associated with a complete set of traceless hermitian matrices σ_i:

$$\rho = \frac{1}{N}(I + \overrightarrow{v} \cdot \overrightarrow{\sigma}) \tag{2.41}$$

In this space, a dynamical map is in general an affine map [22]. Affine maps are given as a linear transformation A followed by a translation:

$$\overrightarrow{v} \rightarrow A(\overrightarrow{v}) + \overrightarrow{y} \tag{2.42}$$

We can see that an affine map preserves the trace of density matrices since:

$$\rho \to \frac{1}{N}(I + A(\overrightarrow{v}) \cdot \overrightarrow{\sigma} + \overrightarrow{y} \cdot \overrightarrow{\sigma}) \tag{2.43}$$

The matrices σ_i are traceless, so the term that results from the translation vector $\overrightarrow{y}$ does not affect the trace. This is why in this representation we have to consider the set of affine maps rather than just linear transformations.

Given that dynamical maps are affine maps, it is not true that all affine maps are dynamical maps. We have to be careful that arbitrary translations or linear transformations can affect the positivity of the density matrix.

This is best illustrated by considering the example of $N = 2$ density matrices. We know that $N = 2$ density matrices in this vector space is a solid sphere of radius 1, the Bloch sphere. A linear transformation of a sphere gives an ellipsoid. So an affine map for $N = 2$ can be described by a squeezing of the sphere into an ellipsoid, with a rotation, followed by a translation.

If the map takes density matrices to positive matrices of unit trace, then this translated ellipsoid must still lie within the sphere of unit radius (see figure 2.1), because this is a necessary and sufficient condition for the image matrices to be positive.

Therefore, for the map to be dynamical, the amount of translation allowed would depend on the linear transformation of the sphere. The condition for the translated ellipsoid to lie within the sphere can be determined geometrically [22]. Unfortunately, especially in higher dimensions, this condition is very difficult to calculate.

We will also note here that while this geometric condition is necessary for a dynamical map, it is not sufficient. This geometric condition is a sufficient condition for the map to be positive, but not completely positive. The difference between

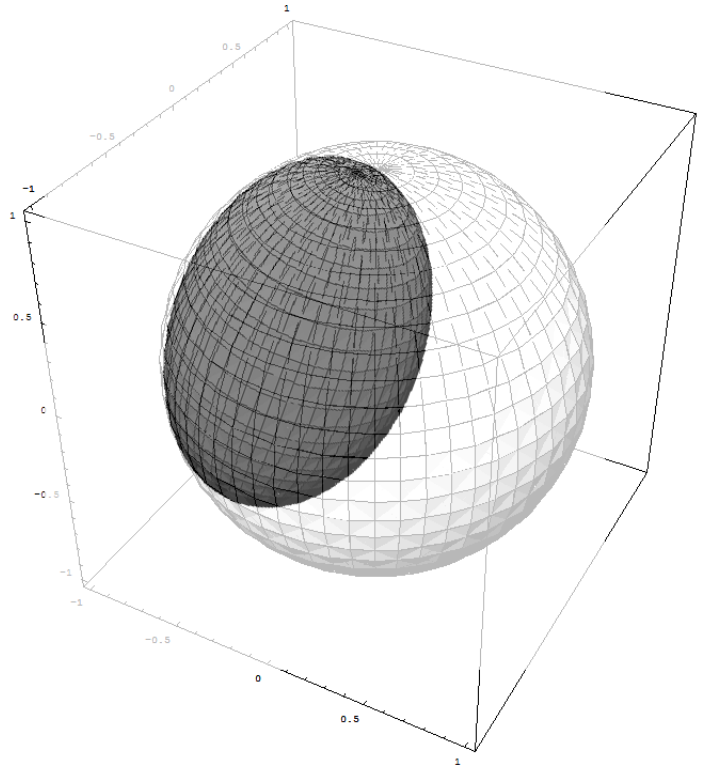

Figure 2.1: Affine map is positive if translated ellipsoid lies within Bloch sphere

positive and completely positive maps will be discussed in a later chapter.

Chapter 3

Quantum measurements

We will begin this chapter by reviewing von Neumann measurements [10] and POVMs [12, 13]. We then present our work on generalized measurements [1], where we show that by suitably extending the system, any linear measurement scheme can be reduced to a unitary transformation and one von Neumann measurement.

3.1 Von Neumann measurements

Let us take a quick refresher on the principles of quantum measurement as outlined by von Neumann [10]. Suppose the quantum system $|\phi\rangle$ is to be measured, and the measurement we wish to perform is given by the operator $Q = \sum_i q_i |i\rangle\langle i| = \sum_i q_i P_i$, where $|i\rangle$ are the eigenvectors for the measurement operator, and P_i are the respective projection operators. Since $|i\rangle$ form a complete basis, we can take the spectral decomposition $|\phi\rangle = \sum_i \alpha_i |i\rangle$.

The system is brought to interact with a macroscopic measuring apparatus, that is initially in the state $|M\rangle$. As the apparatus performs the measurement, the system and apparatus evolves unitarily from the state $\sum_i \alpha_i |i\rangle|M\rangle$ to the state

$\sum_i \alpha_i |i\rangle|M_i\rangle$. In the final step of the measurement, the system and apparatus collapses into the state $|j\rangle|M_j\rangle$ for some value j, and the measurement apparatus registers outcome j. The probability that the system collapses to this state is given by $\langle\phi|P_j|\phi\rangle = |\alpha_j|^2$.

While this measurement process is straightforward, the final collapse of the state is non-linear and indeterminate. We will not be discussing the nature of this collapse. In this chapter, our intent is to work with the basic von Neumann measurement and generalize it within the framework that we had established with density matrices and maps.

Before we proceed further we would like to slightly recast the von Neumann measurement with density matrices instead of rays. Let the quantum system to be measured be given by the density matrix ρ, and the measurement be given by a set of orthornormal projections P_i. When the measurement is performed, the probability of the measurement registering outcome j is $Tr[\rho P_j]$. If the outcome j is observed, then the system collapses to state:

$$\rho \rightarrow \frac{\rho P_j}{Tr[\rho P_j]} \tag{3.1}$$

Notice that here we have omitted the apparatus as well as the measurement operator Q. We are simply interested in the probabilities and the collapsed states, for which the apparatus is mathematically unimportant. Similarly the operator Q is only relevant in that it provides us with a set of orthonormal projections, the eigenvalues of the operator will only be useful if we would like to calculate the expectation value of the operator.

Finally we note that if the measurement is performed over an ensemble, the expected value of the density matrix representing the ensemble following the

measurement would be:

$$\rho \to \sum_i Tr[\rho P_i] \frac{\rho P_i}{Tr[\rho P_i]} = \sum_i \rho P_i \tag{3.2}$$

3.2 POVMs

Positive Operator Value Measure (POVM) [12, 13] is the first generalization of the von Neumann measurement. As with the situation with describing states as rays, problems arise when we try to describe a measurement of an open system. Consider the following example: we have a 2 qubit system, the first qubit is in the state ρ, and the second qubit is in the state $q|0\rangle + (1-q^2)|1\rangle$. We perform a measurement given by the following orthornormal rays:

$$\begin{aligned} &|v_1\rangle \otimes |0\rangle \\ &|v_2\rangle \otimes |0\rangle \\ &|v_3\rangle \otimes |1\rangle \\ &|v_4\rangle \otimes |1\rangle \end{aligned} \tag{3.3}$$

where $\langle v_2|v_1\rangle = 0$ and $\langle v_4|v_3\rangle = 0$.

This measurement has 4 possible outcomes, the probabilities of the respective outcomes are given by:

$$\begin{aligned} &Tr[\rho q^2 |v_1\rangle\langle v_1|] \\ &Tr[\rho q^2 |v_2\rangle\langle v_2|] \\ &Tr[\rho (1-q^2) |v_3\rangle\langle v_3|] \\ &Tr[\rho (1-q^2) |v_4\rangle\langle v_4|] \end{aligned} \tag{3.4}$$

With respect to just the first qubit ρ, we can consider this to be a measure-

ment with the following operators:

$$\begin{aligned} P_1 &= q^2|v_1\rangle\langle v_1| \\ P_2 &= q^2|v_2\rangle\langle v_2| \\ P_3 &= (1-q^2)|v_3\rangle\langle v_3| \\ P_4 &= (1-q^2)|v_4\rangle\langle v_4| \end{aligned} \tag{3.5}$$

These operators will give the correct results: the probability of outcome j is $Tr[\rho P_j]$. If outcome j is observed, the state of the first qubit would be given by:

$$\frac{P_j\rho}{Tr[P_j\rho]} \tag{3.6}$$

But these operators P_i are not orthonormal projections. So for an open system, we find that we need not be constrained to use only orthonormal projections.

Let us revisit our fundamental requirements for a quantum measurement. Instead of orthonormal projections, we could in general allow a set of linear operators to define our measurement. But there are certain conditions these operators have to satisfy. If we follow that the probability of an outcome j is given by $Tr[P_j\rho]$, then P_j should be a positive operator. In addition the sum of probabilities for all outcomes $\sum_i Tr[P_i\rho]$ cannot be greater than 1. If outcome j is observed, and the state of the system is collapsed to the form given by equation 3.6, then the operators should also be hermitian.

Hence we have Positive Operator Value Measure, in this generalized form of measurement all we require is a set of positive hermitian operators P_i that satisfies $\sum_i P_i \leq I$. In most situations it is simpler to require that the operators actually sum to I instead of being an inequality, and this can be easily accomplished by adding the operator $I - \sum_i P_i$ to the list of measurement operators.

In our example above, our set of operators was derived from a set of orthonormal projections in a larger system. Is this always the case? Neumark proved that any set of POVMs can always be given by a set of orthonormal projections in a larger system. We will prove this in the next section as part of a more general result.

While POVMs may seem to magically allow measurements in non-orthogonal directions, we notice that we traded that ability for reduced probabilities. Since the operators must satisfy $\sum_i P_i \leq I$ and each operator is positive, if they are not linearly independent then their norms have to be less than 1. In our example, if the first qubit was in the state $\rho = |v_1\rangle\langle v_1|$, the probability of obtaining the first outcome is only $q^2 \leq 1$. On the other hand if this was a traditional von Neumann measurement and ρ coincided with one of the projections, the probability of obtaining that outcome would have been 1.

So it may appear that we have gained nothing through the complication of POVMs. In fact if we were making measurements over a large ensemble, so that we can reasonably determine the probabilities, then any POVM result can be linearly derived from a von Neumann measurement, or vice versa. So long as the measurement projections or POVMs span the density matrix, then the density matrix can be uniquely determined through any measurement process. The difference between a von Neumann measurement or POVM in this case, is simply a different choice of tomographic reconstruction.

However in situations where a single particle is measured, and that single outcome is of interest, POVMs can be beneficial. POVMs are used often in quantum cryptography and quantum communications where, depending on the desired objective of the measurement, using POVMs may provide a practical advantage over

traditional von Neumann measurements.

3.3 Maps as measurements

In this section we take the final step towards generalizing measurements to not just positive operators, but positive maps.

In the example of an open system we gave in the last section, the second qubit we used could simply be considered part of the apparatus. In fact, we could devise a much more elaborate measurement apparatus. In addition to introducing ancillary particles, we could, for example, perform transformations before and after the state collapse. We could also convexly combine or split operators, to consolidate or create more measurement outcomes.

If we consider the measuring apparatus as a black box, then all we know is that when we feed a particle to the apparatus, one of several possible outcomes is registered, and the particle leaves the apparatus in a different state. However, other than the collapse of the state, all the manipulations within the apparatus would have to be linear. The probability of an outcome should be linearly related to the input state of the system. For a particular outcome, the final state of the system should be given by a linear transformation of the input state.

We know that the most general linear operation on a density matrix is a dynamical map. Therefore we can frame the most general measurement as follows: given a quantum system in state ρ, let the measurement be defined by a set of maps given by their B-matrices $\mathcal{B}^{(i)}$. The probability of registering the jth outcome is $Tr[\mathcal{B}^{(j)}(\rho)]$. If the jth outcome is observed, the final state of the system collapses to:

$$\rho \to \frac{\mathcal{B}^{(j)}(\rho)}{Tr[\mathcal{B}^{(j)}(\rho)]} \tag{3.7}$$

For the probabilities to be positive, the maps would have to be positive. Each map would in general not preserve the trace of the density matrix, otherwise the probability of that outcome would be trivially 1 by our definition. However, the sum of the maps $\sum_i \mathcal{B}^{(i)}$ must reduce or preserve the trace, this is the requirement that the sum of probabilities sum to ≤ 1. Again it is simpler if we simply require that the probabilities sum to 1, by completing the set of maps through adding the map $I - \sum_i \mathcal{B}^{(i)}$.

If the measurement is performed on an ensemble, the expected value for the density matrix representing the ensemble after the measurement is $\sum_i \mathcal{B}^{(i)}(\rho)$.

Now that we have established this elaborate scheme for measurements, we will prove that everything can be accomplished with a unitary transformation and von Neumann measurement, using an ancillary system of sufficient size. This is similar to the method employed in the last chapter with dynamical maps. Let us decompose each map $\mathcal{B}^{(i)}$ into its canonical form:

$$\mathcal{B}^{(i)}\rho = \sum_\alpha c_\alpha^{(i)} C_\alpha^{(i)} \rho {C_\alpha^{(i)}}^\dagger \tag{3.8}$$

We will require that the overall map $\sum_i \mathcal{B}^{(i)}$ preserves trace, by completing the set of maps as necessary. This condition gives:

$$\sum_{i\alpha} c_\alpha^{(i)} {C_\alpha^{(i)}}^\dagger C_\alpha^{(i)} = I \tag{3.9}$$

Now we define a transformation V, that acts on a larger space consisting of our original system and an ancillary system. Let the original system $\mathbb{A}$ be spanned

by the basis states $|r^{\mathbb{A}}\rangle$, and the ancillary system $\mathbb{BC}$ be spanned by the basis states $|i^{\mathbb{B}}\rangle|\alpha^{\mathbb{C}}\rangle$. We define V as follows:

$$V : |r'^{\mathbb{A}}\rangle|0^{\mathbb{B}}\rangle|0^{\mathbb{C}}\rangle \rightarrow \sum_{r,i,\alpha} \sqrt{c_\alpha^{(i)}}[C_\alpha^{(i)}]_{rr'}|r^{\mathbb{A}}\rangle|i^{\mathbb{B}}\rangle|\alpha^{\mathbb{C}}\rangle \tag{3.10}$$

Note that the size of the ancillary system is bounded by μN^2, since $i^{\mathbb{B}}$ ranges from 1 to μ, where μ is the number of maps $\mathcal{B}^{(i)}$, and $\alpha^{\mathbb{C}}$ ranges from 1 to N^2 since each map $\mathcal{B}^{(i)}$ has at most N^2 C-matrices.

We have not yet defined the transformation V on a complete set of basis states, however for the states on which it is defined, V does preserve orthornormality between those states. We prove this using equation 3.9:

$$\begin{aligned} &\left(\langle r'^{\mathbb{A}}0^{\mathbb{B}}0^{\mathbb{C}}|V^\dagger\right)\left(V|s'^{\mathbb{A}}0^{\mathbb{B}}0^{\mathbb{C}}\rangle\right) \\ &\quad = \textstyle\sum_{ri\alpha} c_\alpha^{(i)}[C_\alpha^{(i)}]^*_{rr'}[C_\alpha^{(i)}]_{rs'} = \delta_{r's'} \end{aligned} \tag{3.11}$$

Since it preserves the orthonormality between these states, V can be made into a valid unitary transformation by suitably completing the transformation. This is identical to the method used in the last chapter, except this is a general convex decomposition rather than a canonical decomposition of the map $\sum_i \mathcal{B}^{(i)}$.

Now the measurement process would proceed as follows: Taking our original system in state ρ, we introduce an ancillary system that is in the initial state $|0^{\mathbb{B}}0^{\mathbb{C}}\rangle\langle 0^{\mathbb{B}}0^{\mathbb{C}}|$. We perform the unitary transformation V on the original plus ancillary system to get:

$$\begin{aligned} \rho' &= V\left(\rho \otimes |0^{\mathbb{B}}0^{\mathbb{C}}\rangle\langle 0^{\mathbb{B}}0^{\mathbb{C}}|\right)V^\dagger \\ &= \textstyle\sum_{rr'ss'ij\alpha\beta} \sqrt{c_\alpha^{(i)}}\sqrt{c_\beta^{(j)}}[C_\alpha^{(i)}]_{rr'}\rho_{r's'}[C_\beta^{(j)}]^*_{ss'}|r^{\mathbb{A}}i^{\mathbb{B}}\alpha^{\mathbb{C}}\rangle\langle s^{\mathbb{A}}j^{\mathbb{B}}\beta^{\mathbb{C}}| \end{aligned} \tag{3.12}$$

We then perform a von Neumann measurement on ancillary system $\mathbb{B}$, given by the set of orthonormal projections $|i^{\mathbb{B}}\rangle\langle i^{\mathbb{B}}|$. The probability of the jth outcome is:

$$Tr[\rho'|j^{\mathbb{B}}\rangle\langle j^{\mathbb{B}}|] = \sum_{rr's'\alpha} c_{\alpha}^{(j)} [C_{\alpha}^{(j)}]_{rr'} \rho_{r's'} [C_{\alpha}^{(j)}]_{rs'}^{*} = Tr[\mathcal{B}^{(j)}(\rho)] \tag{3.13}$$

If the jth outcome is observed, then the original plus ancillary system collapses to the state:

$$\frac{1}{K} \sum_{rr'ss'\alpha\beta} \sqrt{c_{\alpha}^{(j)}} \sqrt{c_{\beta}^{(j)}} [C_{\alpha}^{(j)}]_{rr'} \rho_{r's'} [C_{\beta}^{(j)}]_{ss'}^{*} |r^{\mathbb{A}} j^{\mathbb{B}} \alpha^{\mathbb{C}}\rangle\langle s^{\mathbb{A}} j^{\mathbb{B}} \beta^{\mathbb{C}}| \tag{3.14}$$

where $K = Tr[\mathcal{B}^{(j)}(\rho)]$ normalizes the state.

Finally the measurement is over and the particle exits the apparatus. The state of the system, now outside the apparatus, is given by tracing over the ancillary system $\mathbb{BC}$ that remain inside the apparatus:

$$\rho_{rs} \rightarrow \frac{1}{K} \sum_{\alpha r's'} c_{\alpha}^{(j)} [C_{\alpha}^{(j)}]_{rr'} \rho_{r's'} [C_{\alpha}^{(j)}]_{ss'}^{*} = \frac{[\mathcal{B}^{(j)}(\rho)]_{rs}}{Tr[\mathcal{B}^{(j)}(\rho)]} \tag{3.15}$$

Therefore we accomplished the generalized measurement we set out to perform. We only needed an ancillary system big enough (dimension μN^2), one unitary transformation, and one von Neumann measurement on the $\mathbb{B}$ ancillary system.

In the case where we are dealing with POVMs, the maps for the measurement each have only one C-matrix, the C-matrix being the corresponding POVM operator. Since the maps are singular, the ancillary system $\mathbb{C}$ is unnecessary, so the ancillary system just has to have dimension μ equal to the number of maps or POVMs. This proves Newmark's theorem.

The $\mathbb{C}$ ancillary system is only necessary to provide the generalized linear

transformation of the system as dictated by the maps, the measurement really only takes place in the $\mathbb{B}$ system. It is interesting that any arbitrarily complex measurement, perhaps involving multiple steps of transformations, and von Neumann measurements, can all be reduced to a single unitary transformation and single von Neumann measurement.

Finally we note that this generalized measurement process can be used to realize a trace-reducing map. Suppose the trace-reducing map in question is $\mathcal{B}$. We perform the generalized measurement defined by the maps $\mathcal{B}$ and $I - \mathcal{B}$. If the latter outcome is observed, the system is discarded. Therefore, the expected result is $Tr[\mathcal{B}(\rho)]\frac{\mathcal{B}(\rho)}{Tr[\mathcal{B}(\rho)]} = \mathcal{B}(\rho)$. For example, if a large ensemble of electrons is to be prepared in the state $\mathcal{B}(\rho)$, the electrons are put through the generalized measurement apparatus and divided into 2 sets, one set being $\mathcal{B}(\rho)$ and the other being $(I - \mathcal{B})(\rho)$. The trace of each matrix then represents the fraction of the ensemble that is in that set.

Chapter 4

Quantum Entanglement

Quantum entanglement has been a main focus of our research. We begin by reviewing the concept of entanglement and separability [8, 9, 25], the Peres partial transposition criteria for separability [29] and the connection between separability and 1-positive maps [28].

We then discuss our work on positive but not completely positive maps, where we show that such maps have negative eigen-matrices with Schmidt rank greater than 1 and satisfy certain algebraic conditions [4].

4.1 Entanglement of pure states

Quantum entanglement is a phenomena peculiar to quantum states of two or more particles. The classic example [8] is to consider a singlet state of a system consisting of two spin 1/2 particles (qubits):

$$|\Phi\rangle = \frac{1}{\sqrt{2}}(|0^{\mathbb{A}}1^{\mathbb{B}}\rangle - |1^{\mathbb{A}}0^{\mathbb{B}}\rangle) \tag{4.1}$$

Lets say a measurement is made on the $\mathbb{B}$ particle, the measurement basis given by the projections $|0^{\mathbb{B}}\rangle\langle 0^{\mathbb{B}}|$ and $|1^{\mathbb{B}}\rangle\langle 1^{\mathbb{B}}|$. If the measurement apparatus registers the result corresponding to $|0^{\mathbb{B}}\rangle\langle 0^{\mathbb{B}}|$, then the system would have to be collapsed to the state $|1^{\mathbb{A}}0^{\mathbb{B}}\rangle\langle 1^{\mathbb{A}}0^{\mathbb{B}}|$. A subsequent measurement of the $\mathbb{A}$ particle will always give the result corresponding to $|1^{\mathbb{A}}\rangle\langle 1^{\mathbb{A}}|$. If the $\mathbb{B}$ particle had not been previously measured, the result for $\mathbb{A}$ would have been $|0^{\mathbb{A}}\rangle\langle 0^{\mathbb{A}}|$ with probability $1/2$ and $|1^{\mathbb{A}}\rangle\langle 1^{\mathbb{A}}|$ with probability $1/2$. Therefore it appears that the measurement on the $\mathbb{B}$ particle affects the state of the $\mathbb{A}$ particle. The two particles could be arbitrarily spatially separated, but this effect would have been instantaneous.

This is not really a causal effect, but rather an effect that is due to the two qubit system having non local properties. Entanglement was the term coined by Schrodinger [9] to describe the non-local and correlated nature of such states.

Entanglement is more than an interesting phenomena, recent work has shown that entanglement is useful as a practical resource: entangled states are used in quantum computation [46], quantum communications [44, 45], quantum cryptography [43] and quantum teleportation [47]. In all these processes, the quantum nature of entanglement provides practical results that cannot be duplicated with classical systems. Unfortunately entanglement has been elusively difficult to quantify and identify. In this chapter, we will be discussing methods to identify entanglement in a quantum system.

At first, the problem of identifying entanglement does not appear to be difficult. If we consider pure states, then any state of the following form is not entangled:

$$|\Psi\rangle = |\Psi^{\mathbb{A}}\rangle \otimes |\Psi^{\mathbb{B}}\rangle \otimes \dots \tag{4.2}$$

Each particle is in its own individual state, independent of the other particles.

In other words the state of the system is factorizable into states of its local particles. A measurement on particle $\mathbb{A}$ (given by projection $P^{\mathbb{A}}$) is independent of the outcome of a measurement on particle $\mathbb{B}$ (given by projection $P^{\mathbb{B}}$), because the probabilities multiply:

$$Tr[P^{\mathbb{A}} \otimes P^{\mathbb{B}}|\Psi\rangle\langle\Psi|] = Tr[P^{\mathbb{A}}|\Psi^{\mathbb{A}}\rangle\langle\Psi^{\mathbb{A}}|] \cdot Tr[P^{\mathbb{B}}|\Psi^{\mathbb{B}}\rangle\langle\Psi^{\mathbb{B}}|] \tag{4.3}$$

On the other hand we can identify any state of the following (Schmidt) form as entangled:

$$|\Psi\rangle = \sum_r \alpha_r |\Psi_r^{\mathbb{A}}\rangle \otimes |\Psi_r^{\mathbb{B}}\rangle \otimes \dots \tag{4.4}$$

Such a state cannot be described by its local (individual particle) states, as was proved by Bell [11]. Such pure entangled states can be identified mathematically as follows – if the Schmidt number (the number of non-zero Schmidt coefficients) of the state is greater than one, then the state is entangled.

While the situation with pure states is straightforward, as we will see in the following sections, entanglement for mixed states is considerably more difficult to pin down.

4.2 Entanglement of density matrices

With density matrices, a non-entangled density matrix may be defined in a very similar way to pure states, the following density matrix is factorizable into its local particle states:

$$\rho = \rho^{\mathbb{A}} \otimes \rho^{\mathbb{B}} \otimes \dots \tag{4.5}$$

Any local measurement on one particle is independent of a measurement on the other particles in the system:

$$Tr[P^{\mathbb{A}} \otimes P^{\mathbb{B}} \rho] = Tr[P^{\mathbb{A}} \rho^{\mathbb{A}}] \cdot Tr[P^{\mathbb{B}} \rho^{\mathbb{B}}] \tag{4.6}$$

The probabilities multiply, therefore there is no correlation between the outcomes. Clearly such a state is not entangled.

Unfortunately our problem does not end here. With density matrices, we are dealing with convex sets, so how do we classify a convex combination of these non-entangled states?

$$\rho = \sum_i p_i \rho_i^{\mathbb{A}} \otimes \rho_i^{\mathbb{B}} \otimes \dots \tag{4.7}$$

Such a state can have correlations. For example, let us consider the following state:

$$\rho = \frac{1}{2} |0^{\mathbb{A}} 1^{\mathbb{B}}\rangle\langle 0^{\mathbb{A}} 1^{\mathbb{B}}| + \frac{1}{2} |1^{\mathbb{A}} 0^{\mathbb{B}}\rangle\langle 1^{\mathbb{A}} 0^{\mathbb{B}}| \tag{4.8}$$

If we conduct the same measurement as we had described in the previous section with the singlet state, the results would be identical. If a measurement is made on the $\mathbb{B}$ particle, and the $|0^{\mathbb{B}}\rangle\langle 0^{\mathbb{B}}|$ outcome is registered, then the $\mathbb{A}$ particle has to be in state $|1^{\mathbb{A}}\rangle\langle 1^{\mathbb{A}}|$. Conversely if the $|1^{\mathbb{B}}\rangle\langle 1^{\mathbb{B}}|$ outcome is registered then the $\mathbb{A}$ particle has to be in the state $|0^{\mathbb{A}}\rangle\langle 0^{\mathbb{A}}|$. The measurement outcomes are correlated, but is such a state entangled?

Correlations are not unique to quantum entangled states, correlations occur all the time in classical systems. Let us consider an example. Take a system consisting of a pair of cards, where each card can read either 0 or 1. Suppose there is an

entire ensemble of these card pairs, and each card pair is split so one card is held by observer $\mathbb{A}$ and the other card is held by observer $\mathbb{B}$. Let the card pairs be prepared so that the observers are given randomly either $0^{\mathbb{A}} \otimes 1^{\mathbb{B}}$ or $1^{\mathbb{A}} \otimes 0^{\mathbb{B}}$. Therefore with a random sampling of this ensemble, the outcome of a measurement of the card held by observer $\mathbb{B}$ immediately identifies what card observer $\mathbb{A}$ has, and vice versa.

This example closely parallels the quantum state we were discussing. If we made all our measurements in the $|0\rangle, |1\rangle$ basis, then our quantum state behaves just like the classical one. The quantum system could have been prepared just like the ensemble of cards, instead of card pairs, the ensemble is prepared by taking $|0^{\mathbb{A}}1^{\mathbb{B}}\rangle\langle 0^{\mathbb{A}}1^{\mathbb{B}}|$ and $|1^{\mathbb{A}}0^{\mathbb{B}}\rangle\langle 1^{\mathbb{A}}0^{\mathbb{B}}|$ particle pairs.

Any state that can be written as $\sum_i p_i \rho_i^{\mathbb{A}} \otimes \rho_i^{\mathbb{B}} \otimes \ldots$ can be prepared in a similar fashion. Since such states can be prepared in a classical manner, Werner called such quantum states classically correlated [25], and Werner showed that these classical correlated states always satisfy Bell's inequalities.

The violation of Bell's inequalities by pure entangled states has been perhaps the one result most commonly associated with entanglement. Therefore Werner's classically correlated states are not considered to be entangled, but rather classified as separable [27]. States of the form $\rho = \rho^{\mathbb{A}} \otimes \rho^{\mathbb{B}} \otimes \ldots$ are said to be simply separable.

Conversely, any state that cannot be written in a separable form is defined to be entangled. Therefore, entanglement for density matrices expresses a strictly quantum type of correlation.

We can show that if a density matrix cannot be written in a separable form, then any convex decomposition of that density matrix would have to contain at least one pure entangled state.

First we prove that a separable state can always be decomposed in terms of

pure separable states. A separable state was defined as:

$$\rho = \sum_i p_i \rho_i^{\mathbb{A}} \otimes \rho_i^{\mathbb{B}} \otimes \dots \tag{4.9}$$

But each of the matrices ρ_i can be convexly decomposed in terms of pure states, using its eigen decomposition:

$$\rho = \sum_{i,\mu\nu\dots} p_i \alpha_{i,\mu}^{\mathbb{A}} \alpha_{i,\nu}^{\mathbb{B}} \dots |\Phi_{i,\mu}^{\mathbb{A}}\rangle\langle\Phi_{i,\mu}^{\mathbb{A}}| \otimes |\Phi_{i,\nu}^{\mathbb{B}}\rangle\langle\Phi_{i,\nu}^{\mathbb{B}}| \otimes \dots \tag{4.10}$$

The coefficients satisfy:

$$p_i \alpha_{i,\mu}^{\mathbb{A}} \alpha_{i,\nu}^{\mathbb{B}} \dots \geq 0 \tag{4.11}$$

$$\sum_i p_i \sum_\mu \alpha_{i,\mu}^{\mathbb{A}} \sum_\nu \alpha_{i,\nu}^{\mathbb{B}} \dots = 1 \tag{4.12}$$

Therefore this is a convex sum of pure separable states.

We know that density matrices can be convexly decomposed in terms of pure states, in fact, any convex decomposition of a density matrix can be expanded so that every term is a pure state. We also know that any convex sum of pure separable states is a separable density matrix. Therefore any convex decomposition of an entangled density matrix into pure states must contain at least one term that is a pure entangled state.

By definition separable density matrices form a closed convex set. However, entangled states do not form a convex set. We can take the example of two pure entangled states:

$$|\Phi\rangle = \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle) \tag{4.13}$$

$$|\Psi\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle) \tag{4.14}$$

The following convex sum of these two entangled states is a separable density matrix:

$$\begin{aligned} \rho &= \tfrac{1}{2}|\Phi\rangle\langle\Phi| + \tfrac{1}{2}|\Psi\rangle\langle\Psi| \\ &= \tfrac{1}{2}|01\rangle\langle 01| + \tfrac{1}{2}|10\rangle\langle 10| \end{aligned} \tag{4.15}$$

By definition, entangled states are the density matrices that are not separable, therefore entangled states form the set given by the difference between the convex set of all density matrices and the convex set of separable density matrices.

4.3 Partial transposition

Although we have the definition of separability and entanglement, it is desirable to have a functional way of distinguishing between separable and entangled density matrices. However the fact that separable states form a convex set poses a problem, as we will see a function that can distinguish the boundary of a convex set can be very complicated.

The Peres partial transposition criterion [29] is the most well known criterion for separability. The idea is very straightforward. Let us consider a separable bipartite state:

$$\rho = \sum_i p_i \rho_i^{\mathbb{A}} \otimes \rho_i^{\mathbb{B}} \tag{4.16}$$

Now let us apply a transposition to the state of the $\mathbb{A}$ system, in effect a partial transposition of the state:

$$\rho^{PT} = \sum_i p_i (\rho_i^{\mathbb{A}})^T \otimes \rho_i^{\mathbb{B}} \tag{4.17}$$

This is a linear transformation. We know that the matrices $\rho_i^{\mathbb{A}}$ are hermitian, so the transpose of these matrices $(\rho_i^{\mathbb{A}})^T = (\rho_i^{\mathbb{A}})^*$ are valid, positive, density matrices. Therefore for a separable bipartite system the density matrix ρ^{PT} is always a positive matrix.

On the other hand, let us consider a pure entangled state:

$$|\Phi\rangle = \alpha|00\rangle + \beta|11\rangle \tag{4.18}$$

The density matrix is for this state is:

$$\begin{pmatrix} \alpha^2 & 0 & 0 & \alpha\beta^* \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \alpha^*\beta & 0 & 0 & \beta^2 \end{pmatrix} \tag{4.19}$$

Now we perform a partial transpose on the first system, which is accomplished by interchanging all elements $|0x\rangle\langle 1x|$ with $|1x\rangle\langle 0x|$. We can visualize this by taking the 4×4 matrix as a 2×2 matrix of blocks, then transposing the off-diagonal blocks. So we get:

$$\begin{pmatrix} \alpha^2 & 0 & 0 & 0 \\ 0 & 0 & \alpha^*\beta & 0 \\ 0 & \alpha\beta^* & 0 & 0 \\ 0 & 0 & 0 & \beta^2 \end{pmatrix} \tag{4.20}$$

We can confirm this is no longer a valid density matrix as it is no longer positive. One of the principal 2×2 sub-matrices has a negative determinant:

$$Det \begin{pmatrix} 0 & \alpha^*\beta \\ \alpha\beta^* & 0 \end{pmatrix} = -\alpha^2\beta^2 \tag{4.21}$$

So when this entangled pure state is partially transposed, the result we get is a negative matrix. It is not too difficult to generalize this proof to all pure entangled states. Using the Schmidt decomposition, we can always write any pure entangled state in the form:

$$|\Phi\rangle = \alpha|00\rangle + \beta|11\rangle + \gamma|22\rangle + \ldots \tag{4.22}$$

If we consider just the first 4×4 sub-matrix of the density matrix for this state, and apply the same analysis as before, we can show that partial transposition maps this state to a negative matrix. Therefore all pure entangled states are mapped to negative matrices by partial transposition.

Since partial transposition gives a positive matrix when acting on all separable density matrices, and gives a negative matrix when acting on all pure entangled states, it would seem reasonable to conjecture that if partial transposition acts on an entangled density matrix it would give a negative matrix. After all, any convex decomposition of an entangled density matrix in terms of pure states must contain

at least one term that is a pure entangled state.

Unfortunately this conjecture is not correct. While it is true that any convex decomposition of an entangled density matrix must contain at least one term that is an entangled pure state, this does not guarantee that after the partial transposition, the positive terms (resulting from the separable terms) cannot balance out the negative terms (resulting from the entangled terms). The set of separable pure states linearly (but not convexly) span the space of matrices, so the negative matrices can always be linearly decomposed in terms of separable pure states. With the appropriate terms in the convex sum, it may be possible for the positive separable terms to balance the entangled terms under partial transposition.

So we find that positive partial transposition is a necessary condition for separability, since all separable density matrices will give a positive matrix under partial transposition. However it may not be a sufficient condition for separability.

It was shown in [28] that for a system consisting of two $N = 2$ particles, or one $N = 2$ particle and one $N = 3$ particle, positivity under partial transposition is a necessary and sufficient condition for a state to be separable. We will present this proof in the next section. For higher level systems, specific counter-examples have been given of entangled matrices that have positive partial transpose, therefore partial transposition is not a sufficient condition of separability in general.

4.4 Positive maps as entanglement witnesses

Partial transposition acts linearly on the density matrix, therefore it is a linear map. Partial transposition is not a positive map, since we already have an example where it takes an entangled density matrix to a negative matrix. However transposition (not partial) itself appears to be a positive map, it maps density matrices to valid density

matrices. So the transposition map $\mathcal{T}$ is positive, but the partial transposition map $\mathcal{T} \otimes I$ is not positive.

This is pretty unusual, we would have expected if $\mathcal{T}$ is positive then $\mathcal{T} \otimes I$ should still be positive, since I is clearly positive. This unusual property of positive maps can be codified. A map $\mathcal{B}$ is said to be m-positive if the map $\mathcal{B} \otimes I_m$ is positive. Note that a $(m+1)$-positive map is by definition also m-positive. A map that is m-positive for all m is said to be completely positive.

In general, physical dynamical maps are assumed to be completely positive. If a physical operation on a system is described by a map $\mathcal{B}$, then $\mathcal{B} \otimes I$ representing that physical operation acting on just one part of a bi-partite system, should not give a negative matrix. A negative matrix would imply negative probabilities, so it is not a physical state. Therefore in general we require $\mathcal{B} \otimes I$ to always give positive matrices, which means $\mathcal{B}$ has to be completely positive.

We note that there are certain dynamics of open systems that may be described with non-positive maps [34], however the domain of allowed states in those cases is restricted; the domain of states allowed by such a system is not the complete set of all density matrices. We will discuss this in more detail in the next chapter.

For us, the m-positive but not completely positive maps may be our key to a functional method of distinguishing separable states from entangled states. Transposition is a 1-positive but not a 2-positive map. Transposition is not the only positive but not completely positive map, so perhaps other such maps would help us.

Consider a positive but not completely positive map $\mathcal{B}$. $\mathcal{B} \otimes I$ acting on a separable density matrix would always give a positive matrix:

$$\mathcal{B} \otimes I(\sum_i p_i \rho_i^{\mathbb{A}} \otimes \rho_i^{\mathbb{B}}) = \sum_i p_i \mathcal{B}(\rho_i^{\mathbb{A}}) \otimes \rho_i^{\mathbb{B}} \tag{4.23}$$

Since each term $\mathcal{B}(\rho_i^{\mathbb{A}})$ is a positive matrix, the overall matrix is a positive matrix. So it is a necessary condition for a separable density matrix to remain positive under $\mathcal{B} \otimes I$ for all 1-positive maps $\mathcal{B}$. But what about sufficiency?

The sufficiency of this condition was proved in [28]. To prove sufficiency, we will need to appeal to some properties of convex sets. We know that separable states form a closed convex set, since any convex sum of 2 separable states is by definition separable. But any separable state can also be decomposed in terms of pure separable states. Therefore the hull of the convex set of separable states is the set of all pure separable states.

The geometric Hahn-Banach theorem states that for any closed compact convex set, there exists a set of linear, continuous, functionals that separate the inside of the convex set from the outside of the convex set. Formally, this theorem is stated as follows: given a point o that is outside the convex set, there exists a linear continous functional f such that for all points w that is inside the convex set:

$$f(o) < 0 \leq f(w) \tag{4.24}$$

We can think of these functionals as hyperplanes that are tangential (supported) to the surface of the convex set, the normal vector to the hyperplane pointing towards the inside of the convex set. Each hyperplane separate two half-spaces, one that contains the convex set, the other excludes the convex set. The intersection of all the former half-spaces then give the convex set itself.

For a Hilbert space, any linear continuous functional f can be given by a

vector in the space, so:

$$f(\rho) = Tr[F\rho] \tag{4.25}$$

where F is a hermitian self-adjoint matrix that represents the normal vector to the hyperplane.

We had stated that the functional has to satisfy $f(w) \geq 0$ for all points in the convex set. But we do not need to verify it for all points in the set, we only need to check the points in the hull. If the functional is positive for the points on the hull, then by linearity of the functional, and given that any point in the set is a convex sum (linear sum with positive coefficients) of the points in the hull, then the functional is positive for all points in the set. Conversely, since the points on the hull do belong to the set, if the functional is positive on all points in the set it must be positive for the points in the hull. So it is necessary and sufficient to find the functionals that are positive for the points on the hull. For the convex set of separable states, the hull is given by the set of pure separable states.

So we wish to find all hermitian self-adjoint matrices F such that for all projections $P^{\mathbb{A}}$ and $P^{\mathbb{B}}$, and for some entangled ρ:

$$Tr[F\rho] < 0 \leq Tr[FP^{\mathbb{A}} \otimes P^{\mathbb{B}}] \tag{4.26}$$

Now we want to relate this to positive maps. Consider a map $\mathcal{F}$ and a pure state projection Q

$$Q = \frac{1}{N^2} \sum_{ji} |jj\rangle\langle ii| \tag{4.27}$$

$$\begin{aligned} Tr[\mathcal{F} \otimes I(P^{\mathbb{A}} \otimes P^{\mathbb{B}})Q] &= \mathcal{F}_{rr',ss'} P^{\mathbb{A}}_{r's'} P^{\mathbb{B}}_{ij} Q_{sj,ri} \\ &= \tfrac{1}{N^2} \mathcal{F}_{ir',js'} P^{\mathbb{A}}_{r's'} P^{\mathbb{B}}_{ij} \end{aligned} \tag{4.28}$$

Let the map be given by $\mathcal{F}_{rr',ss'} = N^2 F^T_{rr',ss'}$. We find the following equivalence:

$$Tr[FP^{\mathbb{A}} \otimes P^{\mathbb{B}}] = Tr[\mathcal{F} \otimes I(P^{\mathbb{A}} \otimes P^{\mathbb{B}})Q] \tag{4.29}$$

For the RHS of this equation to be positive for all projections $P^{\mathbb{A}}$ and $P^{\mathbb{B}}$, the map $\mathcal{F}$ cannot be negative. We show this proof by contradiction. Suppose there is some $P^{\mathbb{A}}$ for which $\mathcal{F}(P^{\mathbb{A}})$ is negative. Then there is some $|\phi\rangle = \sum_i \alpha_i |i\rangle$ such that:

$$\langle \phi | \mathcal{F}(P^{\mathbb{A}}) | \phi \rangle < 0 \tag{4.30}$$

If we choose $P^{\mathbb{B}} = \sum_{ij} \alpha_i \alpha_j^* |i\rangle\langle j|$, and given equation 4.27, we get:

$$\begin{aligned} Tr[\mathcal{F} \otimes I(P^{\mathbb{A}} \otimes P^{\mathbb{B}})Q] &= \textstyle\sum_{rsij} [F(P^{\mathbb{A}})]_{rs} P^{\mathbb{B}}_{ij} \delta_{ri} \delta_{sj} \\ &= \langle \phi | \tilde{F}(P^{\mathbb{A}}) | \phi \rangle < 0 \end{aligned} \tag{4.31}$$

Therefore we get a contradiction, equation 4.29 could not be positive for all projections $P^{\mathbb{A}}$ and $P^{\mathbb{B}}$ if the map $\mathcal{F}$ is negative. The map $\mathcal{F}$ has to be positive, though not necessarily completely positive.

Then by the Hahn-Banach theorem, if ρ is not a separable state, there exists a 1-positive map $\mathcal{F}$ which satisfies:

$$Tr[\mathcal{F} \otimes I(\rho)Q] < 0 \tag{4.32}$$

Since Q is a pure projection, the above implies:

$$\mathcal{F} \otimes I(\rho) < 0 \tag{4.33}$$

So we conclude that a state ρ is separable if and only if $\mathcal{F} \otimes I(\rho) \geq 0$ for all 1-positive maps $\mathcal{F}$.

Now that we know 1-positive maps delineate separable density matrices from entangled density matrices, we would want to know more about 1-positive maps.

As we noted earlier, transposition is a 1-positive map. As it turns out, transposition is special in the lower dimensional spaces. Stormer [17] showed that 1-positive maps of 2×2 matrices to 2×2 matrices can always be decomposed in the following form:

$$\mathcal{B} = \mathcal{D} + \mathcal{G} \circ \mathcal{T} \tag{4.34}$$

where $\mathcal{D}$ and $\mathcal{G}$ are completely positive maps, and $\mathcal{T}$ is the transposition map. Woronowicz [21] later extended the result to 1-positive maps of 2×2 to 3×3 matrices. Woronowicz also showed that maps of higher dimensions cannot always be decomposed in this form by providing a counter-example.

Regardless, this decomposability theorem is enough to prove that for bipartite $N = 2$ systems, positive partial transpose is necessary and sufficient for a density matrix to be separable. Since all 1-positive maps can be decomposed according to equation 4.34, the necessary and sufficient condition for a 2×2 density matrix ρ to be separable becomes:

$$(\mathcal{D} + \mathcal{G} \circ \mathcal{T}) \otimes I(\rho) = \mathcal{D} \otimes I(\rho) + \mathcal{G} \otimes I(\mathcal{T} \otimes I(\rho)) \geq 0 \tag{4.35}$$

This has to be satisfied for all completely positive maps $\mathcal{D}$ and $\mathcal{G}$. But since $\mathcal{D}$ and $\mathcal{G}$ are completely positive, the maps $\mathcal{D} \otimes I$ and $\mathcal{G} \otimes I$ are positive. The only way to get a negative term in this equation is if $\mathcal{T} \otimes I(\rho)$ is negative. Therefore $\mathcal{T} \otimes I(\rho) \geq 0$ is necessary and sufficient for ρ to be separable.

For larger dimensional systems, Woronowicz's results imply partial transposition is not enough. We will need to better understand the structure of these positive but not completely positive maps.

4.5 How maps can be positive without being completely positive

In this section, we will try to understand what makes a map positive yet not completely positive. We will show how negative matrix elements in a map $\mathcal{B}$ can be arranged in such a way that when $\mathcal{B}$ acts directly on ρ these elements are hidden, but when $\mathcal{B} \otimes I$ acts on a larger system these elements appear.

To explore the matrix form of $\mathcal{B}$, we will appeal to Jamiolkowski's representation [19] of maps. Recall that the B-matrix form of a map is given by:

$$[\mathcal{B}(\rho)]_{rs} = \mathcal{B}_{rr',ss'}\rho_{r's'} \tag{4.36}$$

Now we define a pure state:

$$|\Phi\rangle = \frac{1}{\sqrt{\nu}} \sum_{r}^{\nu} |r^{\mathbb{A}}\rangle |r^{\mathbb{B}}\rangle \tag{4.37}$$

where ν is the Schmidt rank of the state.

For the purpose of clarity we will call the states $|r^{\mathbb{A}}\rangle$ as the $\mathbb{A}$ Schmidt basis and the states $|r^{\mathbb{B}}\rangle$ as the $\mathbb{B}$ Schmidt basis.

Consider the action of the map $\mathcal{B} \otimes I_\nu$ acting on the state $|\Phi\rangle$. We will find that the resulting density matrix $\mathcal{B} \otimes I(|\Phi\rangle\langle\Phi|)$ is given by a $\nu N \times \nu N$ sub-matrix of $\mathcal{B}$:

$$\mathcal{B} \otimes I(|\Phi\rangle\langle\Phi|) = \frac{1}{\nu} \sum_{rr'ss'} \mathcal{B}_{rr',ss'} |r^{\mathbb{A}} r'^{\mathbb{B}}\rangle\langle s^{\mathbb{A}} s'^{\mathbb{B}}| \tag{4.38}$$

If $\nu = N$ then the result is just the matrix $\mathcal{B}$ itself. We can identify that the eigen-values of this density matrix is the same as the c-values of the map. Also we can associate the eigen-vectors $|\alpha\rangle$ of this density matrix with the C-matrices C_α of the map:

$$|\alpha\rangle = [C_\alpha]_{rs} |r^{\mathbb{A}}\rangle |s^{\mathbb{B}}\rangle \tag{4.39}$$

This simple relationship between maps and $N^2 \times N^2$ density matrices is often called the Jamiolkowski isomorphism. However it is not strictly an isomorphism because maps and density matrices do not have the same trace condition, in addition this relationship does not preserve the multiplicative properties of the maps. The composition of two maps is given by the multiplication of the A-matrices, and not by the multiplication of the B-matrices. In addition it is also not a bijection. If we restrict the discussion to trace preserving completely positive maps, this would only be a subset of all density matrices, since the map has to satisfy the constraint:

$$\sum_r \mathcal{B}_{rr',rs'} = \delta_{r's'} \tag{4.40}$$

If we relax the discussion to include non completely positive maps, which do not have positive B-matrices, then they would also not be good density matrices. Therefore we feel that it is more accurate to call this a representation. The

Jamiolkowski representation is useful because we can now delve into the structure of maps using the familiar language of density matrices, keeping in mind that maps need not follow the same positivity and trace conditions of density matrices.

First we will consider the eigen decomposition of the B-matrix. By Jamiolkowski's representation, the B-matrix of the map is the same as the matrix resulting from $\mathcal{B} \otimes I$ acting on the pure state $\sum_r |r^{\mathbb{A}}\rangle|r^{\mathbb{B}}\rangle$. If the map is completely positive, then this final matrix should be positive. Hence the B-matrix has to be a positive matrix, so all the c-values have to be positive. On the other hand would a positive but not completely positive map have all positive c-values?

First we will show that if the map $\mathcal{B}$ has a negative c-value c_γ, with associated C-matrix C_γ, then $\mathcal{B}$ cannot be $rank(C_\gamma)$-positive.

Let us begin by taking the polar decomposition of C_γ:

$$C_\gamma = U_\gamma M_\gamma \tag{4.41}$$

where $U_\gamma \in SU(N)$ and M_γ is a hermitian matrix. Since M_γ is hermitian, it has an eigen decomposition. Let us denote the eigen-vectors of M_γ as $|r_\gamma\rangle$. Now we define the entangled state:

$$|\Phi\rangle = \frac{1}{\sqrt{\nu}} \sum_r^\nu |r_\gamma^{\mathbb{A}}\rangle|r^{\mathbb{B}}\rangle \tag{4.42}$$

where $\nu = rank(C_\gamma) = rank(M_\gamma)$.

When we act on this state with the map $\mathcal{B} \otimes I_\nu$, the resulting matrix $\mathcal{B} \otimes I(|\Phi\rangle\langle\Phi|)$ is a $\nu N \times \nu N$ sub-matrix of $\mathcal{B}$:

$$\mathcal{B} \otimes I(|\Phi\rangle\langle\Phi|) = \frac{1}{\nu} \sum_{rs}^{N} \sum_{r's'}^{\nu} \mathcal{B}_{rr'_\gamma, ss'_\gamma} |r^{\mathbb{A}} r'^{\mathbb{B}}\rangle\langle s^{\mathbb{A}} s'^{\mathbb{B}}| \tag{4.43}$$

The reason for using the vectors $|r_\gamma\rangle$, is that the domain of C_γ is fully spanned by the vectors $|r_\gamma\rangle$:

$$\sum_r C_\gamma |r_\gamma\rangle\langle r_\gamma| = C_\gamma \tag{4.44}$$

Therefore when we use these vectors, we ensure that a full copy of C_γ is preserved in the resulting matrix:

$$\mathcal{B}_{rr'_\gamma,ss'_\gamma} = c_\gamma [C_\gamma]_{rr'_\gamma} [C_\gamma]^*_{ss'_\gamma} + \sum_{\alpha\neq\gamma} c_\alpha [C_\alpha]_{rr'_\gamma} [C_\alpha]^*_{ss'_\gamma} \tag{4.45}$$

We can think of this as a projection of the matrix $\mathcal{B}$ into the sub-space given by the domain of C_γ. In this projected sub-space, since a full copy of C_γ is preserved, C_γ remains orthogonal to the other C_α, even though the other C_α no longer necessarily form an orthogonal set. Therefore C_γ remains an eigen vector/operator of this projected matrix, and as a result this matrix also inherits the negative eigen-value c_γ.

We conclude that $\mathcal{B}\otimes I_\nu(|\Phi\rangle\langle\Phi|)$ is not positive, therefore $\mathcal{B}$ is not ν-positive.

At the conclusion of this proof, we are beginning to guess how having a negative c-value in the B-matrix does not necessarily prevent a map from being positive. Consider a map $\mathcal{B}$ that has a negative c-value and associated C-matrix that is rank ν. Let $\mathcal{B}\otimes I$ act on a pure entangled state that has Schmidt rank $t<\nu$. In this situation only a $tN\times tN$ sub-matrix of $\mathcal{B}$ is involved. This sub-matrix is not sufficiently large to contain a full copy of the C-matrix that carries that negative c-value. This C-matrix is truncated, so it is no longer orthogonal to the other C-matrices. Consequently its negative c-value can be balanced by the other positive c-values.

This is best demonstrated by an example, which we will provide in our analysis of $N = 2$ positive maps in a later section. But before we get to this analysis, we will need to derive additional results and properties that we will need to complete the analysis.

For the rest of our discussion, to eliminate the cumbersome wording, we will refer to a C-matrix that is associated with a negative c-value, as a negative C-matrix. We note that this does not mean the C-matrix itself is negative. Conversely we will refer to a C-matrix that is associated with a positive c-value as a positive C-matrix.

4.6 More properties of positive but not completely positive maps

4.6.1 Schmidt basis

In the proof given in the last section, we had devised a pure state $|\Phi\rangle$:

$$|\Phi\rangle = \frac{1}{\sqrt{\nu}} \sum_{r}^{\nu} |r_{\gamma}^{\mathbb{A}}\rangle |r^{\mathbb{B}}\rangle \tag{4.46}$$

in order to show that $\mathcal{B} \otimes I(|\Phi\rangle\langle\Phi|)$ is negative. In our construction we used specifically the vectors $|r_\gamma\rangle$ to ensure that we span the domain of C_γ, in order for C_γ to be an eigen-vector/operator of the resultant matrix.

Instead of using $|r_\gamma\rangle$, we notice that any set of orthonormal vectors with the same span would have accomplished the same effect. We also notice that the $\mathbb{B}$ Schmidt basis could be completely arbitrary. Therefore we can state that if a pure state $|\Psi\rangle$ has the same $\mathbb{A}$ Schmidt basis span as $|\Phi\rangle$, then $\mathcal{B} \otimes I(|\Psi\rangle\langle\Psi|) < 0$ if $\mathcal{B} \otimes I(|\Phi\rangle\langle\Phi|) < 0$.

4.6.2 Schmidt coefficients

In the proof of the last section we had also defined our state with completely degenerate Schmidt coefficients. This degeneracy gave us a direct sub-matrix of the B-matrix as the result of $\mathcal{B} \otimes I(|\Phi\rangle\langle\Phi|)$. But we can demonstrate that if the pure state did not have degenerate Schmidt coefficients, it would not have affected the positivity or negativity of the resulting matrix.

Suppose we had used the following state with Schmidt coefficients α_r:

$$|\Phi\rangle = \sum_{r}^{\nu} \alpha_r |r_\gamma^{\mathbb{A}}\rangle |r^{\mathbb{B}}\rangle \tag{4.47}$$

where $\alpha_r \neq 0$. We will not consider the case where $\alpha_r = 0$ since that will reduce the Schmidt rank of the state, which will alter the problem we are discussing.

The map $\mathcal{B} \otimes I$ acting on this state gives the resulting matrix:

$$\alpha_{r'} \alpha_{s'}^* \mathcal{B}_{rr'_\gamma, ss'_\gamma} \tag{4.48}$$

Suppose that $\mathcal{B}_{rr',ss'}$ is negative, then there is some vector x such that:

$$x_{rr'}^\dagger \mathcal{B}_{rr',ss'} x_{ss'} < 0 \tag{4.49}$$

We can define a new vector $y_{rr'} = \alpha_{r'}^{-1} x_{rr'}$ which would satisfy:

$$y_{rr'}^\dagger (\alpha_{r'} \alpha_{s'}^* \mathcal{B}_{rr'_\gamma, ss'_\gamma}) y_{ss'} < 0 \tag{4.50}$$

Therefore the Schmidt coefficients do not change whether the resulting matrix is positive or negative.

4.6.3 Schmidt rank N states

We can show that if a map $\mathcal{B}$ is not completely positive, then $\mathcal{B} \otimes I$ acting on any Schmidt rank N pure state will always give a negative matrix.

We will use some of the results we just found. For a Schmidt rank N pure state, the $\mathbb{A}$ Schmidt basis must be complete. Therefore all Schmidt rank N pure states have the same span for the $\mathbb{A}$ Schmidt basis. In addition we also know that the Schmidt coefficients do not alter the outcome. Therefore since $\mathcal{B} \otimes I$ gives a negative matrix when acting on this state:

$$|\Phi\rangle = \frac{1}{N} \sum_{r}^{N} |r^{\mathbb{A}}\rangle |r^{\mathbb{B}}\rangle \tag{4.51}$$

then it will give a negative matrix for all other Schmidt rank N pure states.

4.6.4 Complete positivity

We will show is that the following statements are equivalent:

- A map $\mathcal{B}$ is completely positive
- $\mathcal{B}$ is N-positive
- The B-matrix of $\mathcal{B}$ is positive.

The equivalence between the first and second statement was proved in [18], and the equivalence between the first and third statement was given in [22]. We will provide an alternate proof here with the construction we established in the last section.

Consider the positivity of $\mathcal{B} \otimes I_\nu$ where $\nu > N$. Any pure state of this space can have a maximum Schmidt decomposition of only N terms. Therefore $\mathcal{B}$ is ν-

positive if it is positive on all Schmidt rank N pure states. This by definition means $\mathcal{B}$ is N-positive. Therefore N-positivity is necessary and sufficient for complete positivity. This proves the equivalence between the first and second statement.

We had also showed that if $\mathcal{B}$ is N-positive, then $\mathcal{B} \otimes I$ must be positive on the state $|\Phi\rangle = \frac{1}{N}\sum_r |r^{\mathbb{A}}\rangle|r^{\mathbb{B}}\rangle$, and therefore the $\mathcal{B}$ matrix itself must be positive. Conversely if the map $\mathcal{B}$ is N-positive, then by definition it will be positive on all Schmidt rank N pure states. This proves the equivalence between the second and third statement.

4.6.5 Algebraic condition for positivity

Finally, we want to write down an algebraic condition for a map to be ν-positive. The necessary and sufficient condition that the map is ν-positive is that it must be positive on all Schmidt rank ν pure states. We know that the Schmidt coefficients do not alter the outcomes, so we can just check states with degenerate Schmidt coefficients. For $\nu < N$, we will need to make sure we check states with the $\mathbb{A}$ Schmidt basis covering different spans. So we can write down a pure state with degenerate Schmidt coefficients and generic $\mathbb{A}$ Schmidt basis as follows:

$$|\Phi\rangle = \frac{1}{\sqrt{\nu}} \sum_{r}^{\nu} \sum_{k}^{N} U_{kr} |k^{\mathbb{A}}\rangle |r^{\mathbb{B}}\rangle \tag{4.52}$$

where $U \in SU(N)$. By varying U we can cover all possible spans of the $\mathbb{A}$ Schmidt basis.

Now if we consider $\mathcal{B} \otimes I$ acting on this state, it gets mapped to:

$$\mathcal{B} \otimes I(|\Phi\rangle\langle\Phi|) = \frac{1}{\nu} \sum_{kk'll'}^{N} \sum_{r's'}^{\nu} \mathcal{B}_{kk',ll'} U_{k'r'} U^*_{l's'} |k^{\mathbb{A}} r'^{\mathbb{B}}\rangle\langle l^{\mathbb{A}} s'^{\mathbb{B}}| \tag{4.53}$$

Therefore the following matrix has to be positive:

$$\sum_{kk'll'}^{N} \sum_{r's'}^{\nu} U_{k'r'} \mathcal{B}_{kk',ll'} U^*_{l's'} \tag{4.54}$$

Notice that the indices r', s' only go up to ν. Let us define a ν-dimensional projection:

$$P \equiv \sum_{r}^{\nu} |r\rangle\langle r| \tag{4.55}$$

We can now state that a map $\mathcal{B}$ is ν-positive if and only if for all $U \in SU(N)$:

$$(I \otimes (PU))\mathcal{B}(I \otimes (PU)^\dagger) \geq 0 \tag{4.56}$$

4.7 N=2 1-positive maps

We can apply the results from the previous sections to the analysis of $N = 2$ positive maps, independently of Stormer and Woronowicz results. We find that we can arrive at the same result with just some simple algebra.

Let us use the Jamiolkowski representation for the map, and treat it like a density matrix. For a 2×2 density matrix, we can define the following general eigen-values and eigen-vectors:

$$\begin{array}{ll} W & w|00\rangle + x|11\rangle \\ X & x^*|00\rangle - w^*|11\rangle \\ Y & y|01\rangle + z|10\rangle \\ Z & z^*|01\rangle - y^*|10\rangle \end{array} \tag{4.57}$$

We can write out the matrix given by these eigen-values and eigen-vectors:

$$\begin{pmatrix} Ww^2+Xx^2 & 0 & 0 & (W-X)wx^* \\ 0 & Yy^2+Zz^2 & (Y-Z)yz^* & 0 \\ 0 & (Y-Z)y^*z & Yz^2+Zy^2 & 0 \\ (W-X)w^*x & 0 & 0 & Wx^2+Xw^2 \end{pmatrix} \tag{4.58}$$

We know that for $N = 2$, if the map is 1-positive the rank of the negative C-matrices must be 2. In the Jamiolkowski representation, that is equivalent to stating that the negative eigen-vectors (C-vectors) must have Schmidt rank 2.

Note that we will be using the terms C-vectors and C-matrices interchangeably, the C-vector is simply the vector representation of the C-matrix in the Jamiolkowski representation, as given by equation 4.39.

We can show that a 1-positive map for $N = 2$ can have only one negative c-value by process of elimination. First let us consider the case if the map has 3 negative c-values.

The criteria for the map $\mathcal{B}$ to be 1-positive is:

$$(I \otimes (PU))\mathcal{B}(I \otimes (PU)^\dagger) > 0 \quad \text{for all } U \in SU(2) \tag{4.59}$$

where $P = \sum_r^1 |r\rangle\langle r| = |0\rangle\langle 0|$

For $U = 1$ we have two necessary conditions for 1-positivity:

$$\begin{aligned} Ww^2 + Xx^2 \geq 0 \\ Yy^2 + Zz^2 \geq 0 \end{aligned} \tag{4.60}$$

We can see that if any 3 of the c-values W, X, Y or Z are negative, these inequalities cannot be simultaneously satisfied. Therefore with 3 negative c-values,

the map cannot be 1-positive.

Next let us consider if it is possible for 2 c-values to be negative. From the above inequalities, we know that no pair of coefficients W,X or Y,Z can be negative. So we only need to consider the possibility where one coefficient of each pair W,X and Y,Z is negative. Using the same matrix above and a generic unitary transformation we define as:

$$\begin{aligned} U|0\rangle &= a|0\rangle + b|1\rangle \\ U|1\rangle &= b^*|0\rangle - a^*|1\rangle \end{aligned} \tag{4.61}$$

The matrix $(I \otimes PU)\mathcal{B}(I \otimes PU)^\dagger$ becomes:

$$\begin{pmatrix} (Ww^2 + Xx^2)a^2 & (W-X)wx^*ab \\ (W-X)w^*xa^*b^* & (Wx^2 + Xw^2)b^2 \end{pmatrix} + \begin{pmatrix} (Yy^2 + Zz^2)b^2 & (Y-Z)yz^*a^*b^* \\ (Y-Z)y^*zab & (Yz^2 + Zy^2)a^2 \end{pmatrix} \tag{4.62}$$

A calculation of the determinant of each matrix tells us each matrix term in that sum is negative. For the sum of two negative rank 2 matrices to be positive, the positive eigen-vector of one matrix must balance the negative eigen-vector of the other. However the unitary transformation U transforms the 2 matrices differently, therefore the matrices could not balance for all U unless the matrices are invariant under U. This would mean the matrices are proportional to I contradicting the requirement that 2 eigen-values are negative. Therefore we conclude that for $N = 2$, a 1-positive map can have only one negative c-value.

The best example of a 1-positive map for $N = 2$ is the transposition map $\mathcal{T}$.

The transposition map has the following c-values and C-matrices:

$$\begin{array}{cc} \frac{1}{2} & I_2 \\ \frac{1}{2} & \sigma_x \\ \frac{1}{2} & \sigma_z \\ -\frac{1}{2} & \sigma_y \end{array} \tag{4.63}$$

Since σ_y is rank 2, transposition is not 2-positive. However having a negative c-value does not prevent $\mathcal{T}$ from being 1-positive. We can see that transposition is an extremal solution to the 1-positivity condition. We substitute $w = x = y = z = 1$ and $W = X = Y = \frac{1}{2}, Z = -\frac{1}{2}$ into equation 4.62, and we get:

$$\begin{pmatrix} a^2 & 0 \\ 0 & b^2 \end{pmatrix} + \begin{pmatrix} 0 & a^*b^* \\ ab & 0 \end{pmatrix} \tag{4.64}$$

This matrix has a zero determinant for all values of a and b. If we had started with a negative C-matrix σ_y, and sought an extremal solution to the positivity inequality, then this would have been our solution.

In general the negative C-matrix need not be given by σ_y. However we can show that if the map has only one negative C-value, then any solution $\mathcal{B}$ to the positivity criteria can be decomposed in terms of transposition in the following manner:

$$\mathcal{B} = \mathcal{D} + \mathcal{G} \circ \mathcal{T} \tag{4.65}$$

where $\mathcal{D}$ and $\mathcal{G}$ are completely positive maps.

Suppose our map $\mathcal{B}$ has the following negative C-vector:

$$\alpha|\phi\phi\rangle - \beta|\psi\psi\rangle \tag{4.66}$$

First we will prove that the particular Schmidt basis for this one C-vector does not matter. The positivity criterion is:

$$(I \otimes PU)\mathcal{B}(I \otimes PU)^\dagger \geq 0 \quad \text{for all } U \in SU(N) \tag{4.67}$$

Let us introduce two unitary transformations $V, W \in SU(N)$ such that:

$$\mathcal{B} \rightarrow (V \otimes W)\mathcal{B}(V \otimes W)^\dagger \tag{4.68}$$

The positivity criterion becomes:

$$\begin{aligned}&(V \otimes PUW)\mathcal{B}(V \otimes PUW)^\dagger = \\ &\quad (V \otimes I)(I \otimes P\tilde{U})\mathcal{B}(I \otimes P\tilde{U})^\dagger(V \otimes I)^\dagger \geq 0 \quad \text{for all } \tilde{U} \in SU(N)\end{aligned} \tag{4.69}$$

The unitary transformation $V \otimes I$ does not affect the positivity of the inner matrix. Therefore any product unitary transformation of the matrix $\mathcal{B}$ will not change whether the map is positive.

Since this is the case, we can pick our Schmidt basis in such a way that it is convenient for us. Therefore let us begin with the following negative C-vector instead:

$$\alpha|\phi\phi\rangle - \beta|\psi\psi\rangle \rightarrow \alpha|01\rangle - \beta|10\rangle \tag{4.70}$$

Let us write this in the C-matrix form:

$$\begin{pmatrix} 0 & \alpha \\ -\beta & 0 \end{pmatrix} \tag{4.71}$$

Now let us define the map $\mathcal{G}$ as having only one c-value of 1, and one C-matrix given by:

$$C^{\mathcal{G}} = \begin{pmatrix} \alpha & 0 \\ 0 & \beta \end{pmatrix} \tag{4.72}$$

This map is by definition completely positive. Now if we multiply this C-matrix with σ_y, we get:

$$C^{\mathcal{G}}\sigma_y = \begin{pmatrix} 0 & \alpha \\ -\beta & 0 \end{pmatrix} \tag{4.73}$$

We see that $C^{\mathcal{G}}\sigma_y$ is equivalent to the C-matrix in equation 4.71. Therefore instead of seeking a solution for a map with negative C-matrix of the form given in equation 4.71 , we could instead find a solution for a map with negative C-matrix σ_y. This solution composed with the map $\mathcal{G}$ gives us a 1-positive map with the negative C-matrix we started with.

As the final step, we note that the transposition map contains the minimum C-matrices needed to balance the negative C-matrix σ_y under the positivity criterion. Clearly any larger c-values for I_2, σ_x, σ_z could be separated out to form another completely positive map. Therefore any 1-positive map for $N = 2$, that has a negative C-matrix σ_y, can always be given by:

$$\mathcal{E} + \mathcal{T} \tag{4.74}$$

where $\mathcal{E}$ is completely positive.

Combining the results, we arrive at the form we started out to prove:

$$\mathcal{G} \circ (\mathcal{E} + \mathcal{T}) = \mathcal{D} + \mathcal{G} \circ \mathcal{T} \tag{4.75}$$

where $\mathcal{D} = \mathcal{G} \circ \mathcal{E}$ is completely positive.

Some of these results will help us with finding 1-positive maps of higher dimensions. If the map has only one negative C-matrix, then we can find a solution for the case where the C-matrix has degenerate Schmidt coefficients and a fixed Schmidt basis. The general solution can then be decomposed in terms of this extremal solution in the same fashion.

4.8 Extremal N=3 1-positive maps

In this section we will try to extend the analysis we did in the last section to $N = 3$ positive maps. Unfortunately we have not been completely successful, but the analysis should work in general, though tedious and perhaps requiring numerical methods. Our hope is that once the extremal $N = 3$ 1-positive maps are found, we will be able to observe a pattern to help us to find extremal 1-positive maps for higher dimensions. Ultimately, perhaps we can devise a finite number of tests for separability.

A $N = 3$ 1-positive map can have either rank 2 or rank 3 C-matrices with negative c-values. We begin with considering the case where the map has one rank 3 C-matrix with negative c-value of -1 (let us ignore the overall normalization of the map for now), let that C-matrix be given by the following C-vector (using Jamiolkowski's representation):

$$|00\rangle + |11\rangle + |22\rangle \tag{4.76}$$

We are working with degenerate Schmidt coefficients given our conclusions in the end of the last section. Unfortunately given this one negative C-matrix, there are many solutions to the 1-positivity condition. We will describe just one extremal solution.

We begin by seeking a solution to having the matrix $(I \otimes P)\mathcal{B}(I \otimes P) \geq 0$. One solution is to include the following positive c-values and C-vectors:

$$\begin{array}{ll} \frac{3}{4} & |00\rangle - |11\rangle \\ \frac{1}{4} & |00\rangle + |11\rangle - 2|22\rangle \end{array} \tag{4.77}$$

Now we test the more general condition for $(I \otimes PU)\mathcal{B}(I \otimes U^\dagger P) \geq 0$. First we write a generic unitary transformation U for $N = 3$ as:

$$U = \begin{pmatrix} a & d & g \\ b & e & h \\ c & f & i \end{pmatrix} \tag{4.78}$$

Using this transformation, we find that the map cannot be positive with just those positive C-vectors in 4.77 since:

$$(I \otimes PU)\mathcal{B}(I \otimes PU)^\dagger = \frac{3}{2}\begin{pmatrix} 0 & -ad^* & -ag^* \\ & 0 & -dg^* \\ & & 0 \end{pmatrix} < 0 \tag{4.79}$$

We find that we can balance out this matrix so it is positive by adding the following positive C-vectors to our map:

$$\begin{array}{ll} \frac{3}{2} & |01\rangle \\ \frac{3}{2} & |02\rangle \\ \frac{3}{2} & |10\rangle \\ \frac{3}{2} & |12\rangle \\ \frac{3}{2} & |20\rangle \\ \frac{3}{2} & |21\rangle \end{array} \tag{4.80}$$

The matrix becomes:

$$(I \otimes PU)\mathcal{B}(I \otimes PU)^\dagger = \frac{3}{2}\begin{pmatrix} d^2+g^2 & -ad^* & -ag^* \\ & a^2+g^2 & -dg^* \\ & & a^2+d^2 \end{pmatrix} \tag{4.81}$$

This matrix is now positive, therefore the map is 1-positive.

Let us consider how this map transforms a density matrix. We do this by taking each C-matrix and find how they transform the density matrix:

$$C_{r'r}\rho_{rs}C^\dagger_{ss'} \tag{4.82}$$

With this method, we find that this map transforms a density matrix in the following fashion (after suitably normalizing the map):

$$\mathcal{B}: \begin{pmatrix} \rho_{00} & \rho_{01} & \rho_{02} \\ & \rho_{11} & \rho_{12} \\ & & \rho_{22} \end{pmatrix} \rightarrow \begin{pmatrix} \rho_{11}+\rho_{22} & -\rho_{01} & -\rho_{02} \\ & \rho_{00}+\rho_{22} & -\rho_{12} \\ & & \rho_{00}+\rho_{11} \end{pmatrix} \tag{4.83}$$

This map can be simply expressed as:

$$\mathcal{B}(\rho) = Tr[\rho]I - \rho \tag{4.84}$$

We had started with a rank 3 C-matrix which we assigned a negative c-value, and we arrived at this solution using the minimum positive c-values and C-matrices needed to make the map 1-positive. We cannot separate out or reduce any of the positive terms without making the map negative, therefore we cannot decompose this map into a sum of completely positive map $\mathcal{D}$ and 1-positive map $\mathcal{E}$:

$$\mathcal{B} = \mathcal{D} + \mathcal{E} \tag{4.85}$$

Unfortunately it was shown in [30] that this map can be decomposed as:

$$\mathcal{B} = \mathcal{G} \circ \mathcal{T} \tag{4.86}$$

where $\mathcal{T}$ is the transposition map and $\mathcal{G}$ is a completely positive map. This means that $\mathcal{B} \otimes I$ gives a negative matrix only if $\mathcal{T} \otimes I$ gives a negative matrix, so it is covered by partial transposition. The proof of this decomposition of $\mathcal{B}$ can be given as follows:

Let us write out explicitly the 9×9 B-matrix:

$$\mathcal{B} = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \end{pmatrix} \tag{4.87}$$

On inspection we can see this matrix is negative as we expect. But suppose we partial transpose this matrix, we will get:

$$\mathcal{T} \otimes I(\mathcal{B}) = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \tag{4.88}$$

This matrix is positive. Now recall that the 9×9 B-matrix is equivalent to the density matrix given by $\mathcal{B} \otimes I$ acting on a pure entangled state with degenerate Schmidt coefficients:

$$\mathcal{B}_{rr',ss'} = \left[\mathcal{B} \otimes I(\sum_{ij} |ii\rangle\langle jj|) \right]_{rr',ss'} \tag{4.89}$$

Therefore we can write:

$$\mathcal{T} \otimes I \left(\mathcal{B} \otimes I(\sum_{ij} |ii\rangle\langle jj|) \right) \geq 0 \tag{4.90}$$

We can also write this as:

$$(\mathcal{T} \circ \mathcal{B}) \otimes I(\sum_{ij} |ii\rangle\langle jj|) \geq 0 \tag{4.91}$$

This is necessary and sufficient for $\mathcal{T} \circ \mathcal{B}$ to be completely positive. Therefore:

$$\mathcal{T} \circ \mathcal{B} = \mathcal{G} \Rightarrow \mathcal{B} = \mathcal{T} \circ \mathcal{G} \tag{4.92}$$

where $\mathcal{G}$ is completely positive. To get the result we need, we need to place the transposition map on the right:

$$\begin{aligned} \mathcal{T}\left(\mathcal{G}_{rr',ss'}\rho_{r's'}\right) &= \mathcal{G}_{sr',rs'}\rho_{r's'} \\ &= \mathcal{G}_{ss',rr'}\rho_{s'r'} \\ &= \mathcal{G}^*_{rr',ss'}\rho^T_{r's'} \end{aligned} \tag{4.93}$$

$\mathcal{G}^*$ is still a completely positive map, since the c-values are unchanged. Therefore we arrive at the result:

$$\mathcal{B} = \mathcal{G}^* \circ \mathcal{T} \tag{4.94}$$

It is disappointing to find that in this case we do not have a 1-positive map

that provides a new separability criteria. In principle, we should be able to find all extremal maps using this algebraic method, although making sure that all solutions are covered is difficult. Unfortunately at this time we have been unable find an extremal solution that is not decomposable in the form:

$$\mathcal{B} = \mathcal{D} + \mathcal{G} \circ \mathcal{T} \tag{4.95}$$

where $\mathcal{D}$ and $\mathcal{G}$ are completely positive. Given a negative C-matrix to start with, we find that we will need certain positive C-matrices in order to keep the map 1-positive under the condition $(I \otimes PU)\mathcal{B}(I \otimes PU)^\dagger$. The problem is that our solutions always have these positive C-matrices positioned in the part of the matrix that would make the B-matrix positive under partial transposition.

4.9 Future work

Using a combination of the Jamiolkowski representation and Schmidt decomposition of the C-matrices, we have come to understand the structure of positive but not completely positive maps. We find that the positive but not completely positive behavior of a map can be understood from the eigen decomposition of the map B-matrix. Therefore the problem of separability is more amenable through working with 1-positive maps, since we have better tools for dealing with eigen decompositions of a map matrix than with convex decompositions of the density matrix. The difficulty in working with convex decompositions is that there is no specific unique decomposition or even a limit to the number of terms in the decomposition.

We are now beginning to develop an algebraic approach to constructing 1-positive maps. With some of the results here, we have been able to reduce the size

of the problem, such as being able to use degenerate Schmidt coefficients and a fixed Schmidt basis for the negative C-matrix we start with.

The decomposability of most solutions into transposition has been very interesting. This indicates why the Peres partial transposition criterion is so powerful. We believe there should be an algebraic solution to finding 1-positive maps that are not decomposable into transposition. The problem can be stated as follows: we want to find $N \times N$ matrices $\mathcal{B}$:

$$\mathcal{B} < 0 \tag{4.96}$$

that satisfy:

$$(I \otimes PU)\mathcal{B}(I \otimes PU)^{\dagger} \geq 0 \tag{4.97}$$

$$\mathcal{T} \otimes I(\mathcal{B}) < 0 \tag{4.98}$$

These are straightforward algebraic conditions that we should be able to simultaneously solve for. A solution can certainly be found computationally, but if we understand algebraically how both conditions can be satisfied simultaneously, then we have significantly reduced the number of 1-positive maps we need to find, especially in higher dimensions.

Chapter 5

Dynamics of open systems

We begin this chapter by reviewing how initially entangled open systems can lead to dynamical maps that are negative [34]. We will then present our work on extension maps [3] and dynamics of open systems that are initially correlated but not entangled [5].

5.1 Dynamics resulting in non-positive dynamical maps

In an earlier chapter we had said that dynamical maps should be completely positive. Clearly a physical evolution of a system should not take a positive density matrix to a negative matrix, which would give negative probabilities. However implicit in this statement, is the assumption that the map has to be applicable to all density matrices.

This need not be the case. In certain problems, the state of a system may be constrained to a subset of density matrices. In these problems, the dynamical map has to be positive on this subset of density matrices, but need not in general be positive on all density matrices.

This was studied recently in [34]. Here we will first present an example given in that paper, where the map describing the linear evolution of a system is not positive.

Let us consider a bipartite system $\mathbb{AB}$ of two qubits that is evolved through time t by the following Hamiltonian:

$$H = \omega\sigma_3 \otimes \sigma_1 \tag{5.1}$$

where σ_i are the Pauli matrices.

The evolution of the system by this Hamiltonian is given by a unitary transformation:

$$U = e^{-iHt} = cos(\omega t)I - isin(\omega t)\sigma_3 \otimes \sigma_1 \tag{5.2}$$

We are interested in the evolution of the $\mathbb{A}$ system, which is given by:

$$\rho^{\mathbb{A}} = Tr_{\mathbb{B}}[\rho^{\mathbb{AB}}] \rightarrow Tr_{\mathbb{B}}[U\rho^{\mathbb{AB}}U^{\dagger}] \tag{5.3}$$

This evolution is linear, therefore we should be able to write this as a dynamical map $\mathcal{B}$:

$$\mathcal{B}(\rho^{\mathbb{A}}) = Tr_{\mathbb{B}}[U\rho^{\mathbb{AB}}U^{\dagger}] \tag{5.4}$$

Let us write a general form for the density matrix $\rho^{\mathbb{AB}}$ by expanding it in terms of a complete set of $N^2 - 1 = 15$ traceless hermitian matrices:

$$\rho^{\mathbb{AB}} = \frac{1}{4}(I_4 + a_i\sigma_i \otimes I_2 + b_i I_2 \otimes \sigma_i + c_{ij}\sigma_i \otimes \sigma_j) \tag{5.5}$$

Given this, $\rho^{\mathbb{A}}$ is:

$$\rho^{\mathbb{A}} = Tr_{\mathbb{B}}[\rho^{\mathbb{AB}}] = \frac{1}{2}(I + a_i\sigma_i) \tag{5.6}$$

To solve for the map $\mathcal{B}$, we expand the RHS of equation 5.4:

$$\begin{aligned}&\mathcal{B} : \tfrac{1}{2}(I + a_i\sigma_i) \rightarrow \\ &\tfrac{1}{2}(I + cos(2\omega t)a_1\sigma_1 - sin(2\omega t)c_{21}\sigma_1 + cos(2\omega t)a_2\sigma_2 + sin(2\omega t)c_{11}\sigma_2 + a_3\sigma_3)\end{aligned} \tag{5.7}$$

We can interpret this easily as an affine map:

$$\mathcal{B}(\rho^{\mathbb{A}}) = \frac{1}{2}\left(I + (A(\overrightarrow{a}) + \overrightarrow{y}) \cdot \overrightarrow{\sigma}\right) \tag{5.8}$$

where A is a real linear transformation and $\overrightarrow{y}$ is a real vector. By inspection, we see that A describes a squeezing of the Bloch sphere in the $\overrightarrow{\sigma_1}$ and $\overrightarrow{\sigma_2}$ directions by a factor of $cos(2\omega t)$:

$$A = \begin{pmatrix} cos(2\omega t) & 0 & 0 \\ 0 & cos(2\omega t) & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{5.9}$$

and the translation vector $\overrightarrow{y}$ is:

$$\overrightarrow{y} = -sin(2\omega t)c_{21}\overrightarrow{\sigma_1} + sin(2\omega t)c_{11}\overrightarrow{\sigma_2} \tag{5.10}$$

Geometrically we can see that if the translation is not zero, then the line joining anti-podal points on the $\overrightarrow{\sigma_3}$ axis, since the $\overrightarrow{\sigma_3}$ direction is not squeezed, will be partly translated outside the Bloch sphere. Therefore this affine map does not

map positive matrices to positive matrices.

As an example, let the initial state of the $\mathbb{AB}$ system be given by:

$$\begin{aligned} \rho^{\mathbb{AB}} &= \tfrac{1}{2}(|01\rangle + |10\rangle)(\langle 01| + \langle 10|) \\ &= \tfrac{1}{4}\left(I + \sigma_1 \otimes \sigma_1 + \sigma_2 \otimes \sigma_2 - \sigma_3 \otimes \sigma_3\right) \end{aligned} \tag{5.11}$$

For this state, the coefficients $c_{21} = 0$ and $c_{11} = 1$. We allow this system to evolve under the Hamiltonian (equation 5.1), for $t = \frac{\pi}{4\omega}$. We substitute these values into our general solution, to find the dynamical map for system $\mathbb{A}$:

$$\mathcal{B} : \frac{1}{2}(I + a_i\sigma_i) \rightarrow \frac{1}{2}\left(I + \sigma_2 + a_3\sigma_3\right) \tag{5.12}$$

This map $\mathcal{B}$ is not positive since it can map a valid density matrix to a negative matrix:

$$\mathcal{B} : \frac{1}{2}(I + \sigma_3) \rightarrow \frac{1}{2}(I + \sigma_2 + \sigma_3) \tag{5.13}$$

We will be careful to note here that this is a statement about the map $\mathcal{B}$ itself. The actual state of system $\mathbb{A}$ in our example, is given by $\rho^{\mathbb{A}} = Tr_{\mathbb{B}}[\rho^{\mathbb{AB}}] = \frac{1}{2}I$. The mapping of this particular state yields a positive density matrix:

$$\mathcal{B} : \frac{1}{2}I \rightarrow \frac{1}{2}(I + \sigma_2) \tag{5.14}$$

We notice that the variables c_{11} and c_{21} are implicit parameters of the map, even though they are not part of the unitary transformation U. These variables are part of the density matrix $\rho^{\mathbb{AB}}$, and represents correlations in the overall system $\mathbb{AB}$ that is hidden from $\mathbb{A}$ alone.

These implicit parameters are the reason why this map is not positive. We

know that in general for the density matrix $\rho^{\mathbb{AB}}$ to be positive, there must exist constraints between the coefficients a_i and c_{ij} of the density matrix; for given c_{ij}, not all a_i are permitted. So while the map $\mathcal{B}$ is defined on all values of a_i, implicitly the domain for the map is restricted to those values of a_i that are compatible with the c_{ij} parameters in the map. This is called the compatibility domain for the map.

In the following section we will take a different approach to defining the map, that will clearly express this relationship between the map and information in $\rho^{\mathbb{AB}}$.

5.2 Non-positivity understood using extension maps

Our basic problem can be laid out as follows. We wish to consider the linear transformation of system $\mathbb{A}$, a part of system $\mathbb{AB}$ that undergoes a unitary evolution:

$$\mathcal{B}(\rho^{\mathbb{A}}) = Tr_{\mathbb{B}}[U\mathcal{E}(\rho^{\mathbb{A}})U^{\dagger}] \tag{5.15}$$

$\mathcal{E}$ is what we call an extension map, it is a map that takes $N \times N$ matrices to $N^2 \times N^2$ matrices. An extension map should satisfy:

$$Tr_{\mathbb{B}}[\mathcal{E}(\rho^{\mathbb{A}})] = \rho^{\mathbb{A}} \tag{5.16}$$

The reason for using an extension map is so that we can isolate any implicit parameters of $\rho^{\mathbb{AB}}$ within this extension map. The map $\mathcal{B}$ can now be written as a composition of two maps:

$$\mathcal{B} = \mathcal{D} \circ \mathcal{E} \tag{5.17}$$

where the map $\mathcal{D}$ takes $N^2 \times N^2$ matrices to $N \times N$ matrices, and is defined as:

$$\mathcal{D}(M^{\mathbb{AB}}) = Tr_{\mathbb{B}}[UM^{\mathbb{AB}}U^{\dagger}] \tag{5.18}$$

We can establish that $\mathcal{D}$ is completely positive, since for all $X^{\mathbb{ABC}} \geq 0$:

$$\mathcal{D} \otimes I^{\mathbb{C}}(X^{\mathbb{ABC}}) = Tr_{\mathbb{B}}[U^{\mathbb{AB}}X^{\mathbb{ABC}}U^{\mathbb{AB}\dagger}] \geq 0 \tag{5.19}$$

Since $\mathcal{D}$ is always completely positive, we conclude that the map $\mathcal{B}$ is positive if and only if the extension map $\mathcal{E}$ is positive.

We can prove that if the system $\mathbb{AB}$ is in a simply separable state $\rho^{\mathbb{AB}} = \rho^{\mathbb{A}} \otimes \rho^{\mathbb{B}}$, then the evolution of $\mathbb{A}$ is always completely positive because the extension map is completely positive. For a simply separable system, the extension map can be expressed in general as:

$$\mathcal{E}(\rho^{\mathbb{A}}) = \rho^{\mathbb{A}} \otimes \rho^{\mathbb{B}} \tag{5.20}$$

This extension map is completely positive because for all $M^{\mathbb{AC}} \geq 0$:

$$\mathcal{E} \otimes I(M^{\mathbb{AC}}) = M^{\mathbb{AC}} \otimes \rho^{\mathbb{B}} \geq 0 \tag{5.21}$$

Since this extension map is completely positive, we can conclude that any unitary evolution of a simply separable system $\mathbb{AB}$ always gives a completely positive evolution of the system $\mathbb{A}$.

What happens if we want to consider a system $\mathbb{AB}$ that is in a pure entangled state? In this case we find that the extension map has to be either non-linear (for example, purification is a non-linear map), or if the extension map is linear, it can only be positive on a subset of density matrices. To demonstrate, consider any pure entangled state $|\Phi\rangle$. For a pure entangled state of $\mathbb{AB}$, the density matrix of system

$\mathbb{A}$ is always mixed. For example, we could have:

$$\mathcal{E}(\lambda_1|\phi_1\rangle\langle\phi_1| + \lambda_2|\phi_2\rangle\langle\phi_2|) = |\Phi\rangle\langle\Phi| \tag{5.22}$$

If the extension map is linear, then we can expand:

$$\lambda_1\mathcal{E}(|\phi_1\rangle\langle\phi_1|) + \lambda_2\mathcal{E}(|\phi_2\rangle\langle\phi_2|) = |\Phi\rangle\langle\Phi| \tag{5.23}$$

If $\mathcal{E}$ is positive, then the LHS is a convex sum of terms. However the RHS is a pure state, which is not convexly decomposable in terms of other density matrices. With the noted exception where $\mathcal{E}$ is a pin map, we conclude that $\mathcal{E}$ cannot be positive, otherwise we have a contradiction.

The exception where $\mathcal{E}$ is given by a pin map is always a possible solution to this problem. However it is not an interesting solution since $\mathcal{B}$ will also become a pin map. Our objective is to express the final state of system $\mathbb{A}$ as a evolution of its initial state, with a pin map there is no longer any dependence on the initial state of the system.

Consider the example we worked with in the last section. The extension map in that case is:

$$\mathcal{E}\left(\rho = \frac{1}{2}(I + a_i\sigma_i)\right) = \frac{1}{4}(I + a_i\sigma_i \otimes I + b_i I \otimes \sigma_i + c_{ij}\sigma_i \otimes \sigma_j) \tag{5.24}$$

where b_i and c_{ij} are constants of the map. If b_i and c_{ij} are constants, then this map cannot be completely positive, since constraints exist between a_i, b_i and c_{ij} for the matrix to be positive. The values of a_i for which $\mathcal{E}$ gives a positive matrix is the compatibility domain for the map.

To summarize, the purpose of defining the extension map is to clarify any assumptions that are made in the problem about the relation between the states $\rho^{\mathbb{A}}$ and $\rho^{\mathbb{AB}}$. The domain on which the extension map is positive is the compatibility domain of the problem. The evolution or dynamics of the physical process is only applicable on this compatibility domain, even though the map is mathematically (linearly) defined on all density matrices.

5.3 Extension maps for non-positive maps

We now have a few examples of negative maps that arise from perfectly physical situations. It may be interesting to ask the question, can all non-positive maps be expressed as a unitary evolution of an open system, defined by some extension map? In this section we construct a solution to this question.

Let $\mathcal{B}$ be a non-positive map that preserves trace:

$$\sum_r \mathcal{B}_{rr',rs'} = \delta_{r's'} \tag{5.25}$$

We can write the map $\mathcal{B}$ as the difference of two completely positive hermitian maps. Let us write the $\mathcal{B}$ in its canonical decomposition:

$$\mathcal{B} = \sum_\alpha c_\alpha C_\alpha \times C_\alpha^\dagger \tag{5.26}$$

We can group the positive c-value C-matrices, and the negative c-value C-matrices to define:

$$\mathcal{B}^{(+)} = \sum_{\alpha|c_\alpha>0} c_\alpha C_\alpha \times C_\alpha^\dagger \tag{5.27}$$

$$\mathcal{B}^{(-)} = \sum_{\alpha|c_\alpha<0} |c_\alpha| C_\alpha \times C_\alpha^\dagger \tag{5.28}$$

Note that by definition, both $\mathcal{B}^{(+)}$ and $\mathcal{B}^{(-)}$ are completely positive. And we have:

$$\mathcal{B} = \mathcal{B}^{(+)} - \mathcal{B}^{(-)} \tag{5.29}$$

Let us define matrices J and K as follows (this construction was first used in [33]):

$$J_{s'r'} = \sum_r \mathcal{B}^{(+)}_{rr',rs'} \tag{5.30}$$

$$K_{s'r'} = \sum_r \mathcal{B}^{(-)}_{rr',rs'} \tag{5.31}$$

First, we note that the matrix J (and similarly K) is hermitian:

$$J_{s'r'} = \sum_r \sum_{\alpha|c_\alpha>0} c_\alpha [C_\alpha]_{rr'} [C_\alpha]^\dagger_{s'r} = J^*_{r's'} \tag{5.32}$$

Next we note that J cannot be singular if the map $\mathcal{B}$ is trace preserving, since the trace preserving condition is:

$$J - K = 1 \tag{5.33}$$

J and K are partially traced matrices of $\mathcal{B}^{(+)}$ and $\mathcal{B}^{(-)}$, which are both

completely positive. Therefore J and K must be positive. Given $J = 1 + K$ and the matrices are all positive, it follows that J cannot be singular.

However it is possible that K is singular. Since K is positive and hermitian, we can write the canonical decomposition of K:

$$K = \sum_q k_q |\psi_q\rangle\langle\psi_q| \quad ; k_q > 0 \tag{5.34}$$

We define a pseudo-inverse of matrix K as:

$$K^{-1} = \sum_q k_q^{-1} |\psi_q\rangle\langle\psi_q| \tag{5.35}$$

$$K^{-1}K = \sum_q |\psi_q\rangle\langle\psi_q| \tag{5.36}$$

Let us also define an orthornormal set of eigenvectors $|\phi_q\rangle$ spanning the singular subspace of K:

$$K|\phi_q\rangle = 0 \tag{5.37}$$

We can show that $\mathcal{B}^{(-)}$ must destroy all information in this subspace. Let us consider:

$$\begin{aligned} Tr[\mathcal{B}^{(-)}(|\phi_q\rangle\langle\phi_q|)] &= \textstyle\sum_{r,r's'} \mathcal{B}_{rr',rs'}[\phi_q]_{r'}[\phi_q]^*_{s'} \\ &= \textstyle\sum_{r's'} K_{s'r'}[\phi_q]_{r'}[\phi_q]^*_{s'} \\ &= 0 \end{aligned} \tag{5.38}$$

Since $|\phi_q\rangle\langle\phi_q|$ is a positive density matrix, and $\mathcal{B}^{(-)}$ is a completely positive map, it follows that $\mathcal{B}^{(-)}(|\phi_q\rangle\langle\phi_q|)$ is a positive matrix. Therefore if the trace of this

matrix is zero, then the matrix itself must be zero.

Next let us show:

$$\mathcal{B}^{(-)}(|\phi_q\rangle\langle\psi_r|) = \mathcal{B}^{(-)}(|\psi_r\rangle\langle\phi_q|) = 0 \tag{5.39}$$

Let us define the matrices:

$$\begin{aligned} W_{mn} &= \mathcal{B}^{(-)}_{m\phi_q, n\phi_q} \\ X_{mn} &= \mathcal{B}^{(-)}_{m\phi_q, n\psi_r} \\ Y_{mn} &= \mathcal{B}^{(-)}_{m\psi_r, n\psi_r} \end{aligned} \tag{5.40}$$

and the matrix:

$$Z = \begin{pmatrix} W & X \\ X^\dagger & Y \end{pmatrix} \tag{5.41}$$

Z is a submatrix of $\mathcal{B}^{(-)}$ so it is non-negative. We showed that $W = 0$ in equation 5.38, therefore it follows $X = X^\dagger = 0$ otherwise Z would be negative.

This gives us a very useful result:

$$\begin{aligned} \mathcal{B}^{(-)}(\rho) &= \mathcal{B}^{(-)}\left((\textstyle\sum_q |\psi_q\rangle\langle\psi_q| + \sum_u |\phi_u\rangle\langle\phi_u|)\rho\right) \\ &= \mathcal{B}^{(-)}(\Psi\rho) \end{aligned} \tag{5.42}$$

where $\Psi = \sum_q |\psi_q\rangle\langle\psi_q|$.

Now we can move on to the main result – defining an extension map and unitary evolution for a non-positive map $\mathcal{B}$. Let us define the extension map:

$$\mathcal{E}(\rho) = (J\rho) \otimes |e_{(+)}\rangle\langle e_{(+)}| - (K\rho) \otimes |e_{(-)}\rangle\langle e_{(-)}| \tag{5.43}$$

This satisfies the condition:

$$Tr_{\mathbb{B}}[\mathcal{E}(\rho)] = (J-K)\rho = \rho \tag{5.44}$$

We note that the dimension of the space needed for this extended state is $dim(J) + dim(K)$, and $dim(J) = N$ since J cannot be singular.

Then let us define a map $\mathcal{D}$:

$$\mathcal{D}(\rho \otimes |e_{(+)}\rangle\langle e_{(+)}|) = \mathcal{B}^{(+)}(J^{-1}\rho) \otimes |e_{(+)}\rangle\langle e_{(+)}| \tag{5.45}$$

$$\mathcal{D}(\rho \otimes |e_{(-)}\rangle\langle e_{(-)}|) = \mathcal{B}^{(-)}(K^{-1}\rho) \otimes |e_{(-)}\rangle\langle e_{(-)}| \tag{5.46}$$

$\mathcal{D}$ is completely positive since all its components, $\mathcal{B}^{(+)}$, $\mathcal{B}^{(-)}$, J and K, are positive. It is also trace preserving, since for the $(+)$ component:

$$Tr[\mathcal{B}^{(+)}(J^{-1}\rho)] = \mathcal{B}^{(+)}_{rr',rs'} J^{-1}_{r't'} \rho_{t's'} = J_{s'r'} J^{-1}_{r't'} \rho_{t's'} = Tr[\rho] \tag{5.47}$$

For the $(-)$ component, singularities in $\mathcal{B}^{(-)}$ poses a minor problem:

$$Tr[\mathcal{B}^{(-)}(K^{-1}\rho)] = Tr[\Psi\rho] \tag{5.48}$$

However, we note that after applying the extension map the domain of states is $K\rho$, and $\Psi(K\rho) = K\rho$, so this component map is trace preserving on this domain.

Therefore the map $\mathcal{D}$ is completely positive and trace preserving. Putting $\mathcal{D}$ and $\mathcal{E}$ together we have:

$$Tr_{\mathbb{B}}[\mathcal{D}(\mathcal{E}(\rho))] = \mathcal{B}(\rho) \tag{5.49}$$

Since $\mathcal{D}$ is completely positive and trace preserving, we can write it as a uni-

tary transformation of an extended system. The dimension of the ancillary system required is $dim(J) * \mu^{(+)} + dim(K) * \mu^{(-)}$, where $\mu^{(+)}$ and $\mu^{(-)}$ are the number of C-matrices of $\mathcal{B}^{(+)}$ and $\mathcal{B}^{(-)}$ respectively, so $\mu^{(+)} + \mu^{(-)} \leq N^2$.

5.4 Dynamics of an initially non-entangled system that results in non-positive maps

In an earlier section we had come to the conclusion that if the system $\mathbb{AB}$ is in a pure entangled state, the map of system $\mathbb{A}$ is usually a non-positive map. We also concluded that if the system $\mathbb{AB}$ is in a simply separable state, the map of $\mathbb{A}$ is always completely positive. It would be tempting to conjecture that the map of $\mathbb{A}$ is completely positive for all separable states of $\mathbb{AB}$. However this is not true, and in this section we will give an example of a separable system $\mathbb{AB}$ that results in a non-positive map.

Let us begin the system $\mathbb{AB}$ in the following state:

$$\rho^{\mathbb{AB}} = \frac{1}{4}(I_4 + \overrightarrow{a} \cdot \overrightarrow{\sigma} \otimes I_2) + \frac{1}{4}(I_4 + \sigma_2 \otimes \sigma_3) \tag{5.50}$$

This state is separable, which we can prove simply by demonstrating a separation:

$$\begin{aligned} \rho^{\mathbb{AB}} = \quad & \tfrac{1}{8}(I_2 + \overrightarrow{a} \cdot \overrightarrow{\sigma}) \otimes I_2 \\ & + \tfrac{1}{8}(I_2 + \sigma_2) \otimes (I_2 + \sigma_3) + \tfrac{1}{8}(I_2 - \sigma_2) \otimes (I_2 - \sigma_3) \end{aligned} \tag{5.51}$$

The initial state of the system $\mathbb{A}$ is given by:

$$\rho^{\mathbb{A}} = Tr_{\mathbb{B}}[\rho^{\mathbb{AB}}] = \frac{1}{2}I + \frac{1}{4}\overrightarrow{a} \cdot \overrightarrow{\sigma} \tag{5.52}$$

Let us consider the evolution of the $\mathbb{AB}$ system by the following Hamiltonian:

$$H = \omega \sum_i \sigma_i \otimes \sigma_i \tag{5.53}$$

The unitary transformation representing the evolution of the system through time t is given by:

$$U = e^{-iHt} = cos(\omega t)I - isin(\omega t)\sigma_i \otimes \sigma_i \tag{5.54}$$

We can solve algebraically for the state of $\rho^{\mathbb{A}}$ as given by:

$$\rho^{\mathbb{A}} = Tr_{\mathbb{B}}[U\rho^{\mathbb{AB}}U^{\dagger}] \tag{5.55}$$

The calculation is straightforward but lengthy, we notice that most terms can be eliminated when the partial trace is taken over $\mathbb{B}$. We will skip the calculation and show the result:

$$\rho^{\mathbb{A}} \rightarrow \frac{1}{2}I + \frac{1}{4}cos(2\omega t)\overrightarrow{a} \cdot \overrightarrow{\sigma} - \frac{1}{4}sin(2\omega t)\sigma_1 \tag{5.56}$$

Once again the simplest way to describe the map is to use an affine map. By inspection we can see that the affine map is given by:

$$A(\overrightarrow{a}) + \overrightarrow{y} = cos(2\omega t)I_3\overrightarrow{a} - sin(2\omega t)\overrightarrow{\sigma_1} \tag{5.57}$$

where the real linear transformation is a squeezing of the unit sphere into a sphere of radius $cos(2\omega t)$, followed by a translation of magnitude $sin(2\omega t)$ in the $\overrightarrow{\sigma_1}$ direction. Given this, we can derive geometrically that the map is positive only if:

$$|sin(2\omega t)| \leq |cos(2\omega t)| \tag{5.58}$$

Clearly this condition will be violated for certain values of ωt. Therefore the dynamical map for this system can be negative, even though the initial state is separable.

5.5 Zero discord states give positive maps

Consider the situation where a von Neumann measurement, given by an orthonormal set of projections P_i, is made on system $\mathbb{A}$. The state of the overall system $\mathbb{AB}$ collapses to the following state:

$$\gamma^{\mathbb{AB}} \rightarrow P_i \gamma^{\mathbb{AB}} P_i \tag{5.59}$$

We can also write the state in a different form:

$$P_i \gamma^{\mathbb{AB}} P_i = \sum_i p_i P_i \otimes \tau_i \tag{5.60}$$

where $p_i = Tr[P_i \gamma^{\mathbb{AB}}]$ is the probability of obtaining the ith outcome, and $\tau_i = \frac{1}{p_i} Tr_{\mathbb{A}}[P_i \gamma^{\mathbb{AB}}]$ is the normalized state of system $\mathbb{B}$ associated with the ith outcome.

Written in this form, we see that the state is separable but not simply separable, and has the special property that it is a convex sum of matrices that are orthonormal projections in $\mathbb{A}$. Such a density matrix is said to have zero discord [48] [49].

Since the projections P_i are orthonormal, a von Neumann measurement made in the $\mathbb{A}$ system in that particular basis can distinguish between each component in

that convex sum. We can draw a parallel here with a classically correlated system, and consider P_i and τ_i as labels for different classical states of the system $\mathbb{A}$ and $\mathbb{B}$. The state of the system then represents a stochastic mix of such correlated states $P_i \otimes \tau_i$. In a classically correlated system, each state is distinguishable; there is no possibility of a state being a superposition of other states. A quantum separable state, on the other hand, does not have to be a stochastic sum of terms that are distinguishable in any measurement.

Therefore, while all separable states are said to be classically correlated [25], a separable state of the zero discord form would most closely parallel a classically correlated system. From a more practical standpoint, a separable zero discord state is interesting because it is always formed when a von Neumann measurement is performed on an open system.

We know that for an open system that is in a separable but not simply separable state, its evolution is not always given by a completely positive map. However we can show that in this case, when the system is initially measured, the evolution is always given by a completely positive map.

Let us take our initial state as:

$$\rho^{\mathbb{AB}} = \sum_i p_i P_i \otimes \tau_i \tag{5.61}$$

The map $\mathcal{B}$ that describes the evolution of system $\mathbb{A}$ is given by:

$$\mathcal{B}(\rho^{\mathbb{A}}) = Tr_{\mathbb{B}}[U\rho^{\mathbb{AB}}U^{\dagger}] \tag{5.62}$$

Let us expand the RHS:

$$\sum_i p_i U_{r\alpha,r'\alpha'} [P_i]_{r's'} [\tau_i]_{\alpha'\beta'} U^\dagger_{s'\beta',s\alpha} \tag{5.63}$$

We can define a set of maps $\mathcal{B}^{(i)}$:

$$[\mathcal{B}^{(i)}(M^{\mathbb{A}})]_{rs} = \sum_i U_{r\alpha,r'\alpha'} [M^{\mathbb{A}}]_{r's'} [\tau_i]_{\alpha'\beta'} U^\dagger_{s'\beta',s\alpha} \tag{5.64}$$

This will allow us to write:

$$\mathcal{B}(\rho^{\mathbb{A}}) = \sum_i p_i \mathcal{B}^{(i)}(P_i) \tag{5.65}$$

Since P_i are orthonormal, we can express:

$$p_i = Tr[P_i \rho^{\mathbb{A}}] \tag{5.66}$$

which gives us:

$$\mathcal{B}(\rho^{\mathbb{A}}) = \sum_i Tr[\rho^{\mathbb{A}} P_i] \mathcal{B}^{(i)}(P_i) \tag{5.67}$$

Each map $\mathcal{B}^{(i)}$ is by definition completely positive, therefore the matrices $\mathcal{B}^{(i)}(P_i)$ are positive. $Tr[\rho P_i]$ is also always positive if ρ is a valid density matrix, since it represents a probability. Therefore $\mathcal{B}$ is a positive map, since all positive density matrices $\rho^{\mathbb{A}}$ are mapped to a positive sum of positive matrices.

We can prove that the map $\mathcal{B}$ is not just positive, but is completely positive. Let us consider the action of the map again:

$$\begin{aligned}\mathcal{B}(\rho^{\mathbb{A}}) &= \textstyle\sum_i U p_i P_i \otimes \tau_i U^\dagger \\ &= \textstyle\sum_i U \sqrt{\tau_i} p_i P_i \sqrt{\tau_i} U^\dagger \\ &= \textstyle\sum_i V_i p_i P_i V_i^\dagger\end{aligned} \tag{5.68}$$

where $V_i = U\sqrt{\tau_i}$. Let us now exploit the fact that P_i are orthnormal projections, and write:

$$\begin{aligned}\mathcal{B}(\rho^{\mathbb{A}}) &= \textstyle\sum_{ij} V_j p_i \delta_{ij} P_j V_j^\dagger \\ &= \textstyle\sum_{ij} V_j p_i P_j P_i P_j V_j^\dagger \\ &= \textstyle\sum_{ij} C_j p_i P_i C_j^\dagger \\ &= \textstyle\sum_j C_j \rho^{\mathbb{A}} C_j^\dagger\end{aligned} \tag{5.69}$$

What we did here is to exploit the fact that each V_i only acts on P_i, which lies in orthogonal subspaces in the matrix $\rho^{\mathbb{A}}$. Therefore we can define $C_i = V_i P_i$ and combine all elements into a single linear map. The final equation above gives $\mathcal{B}$ in a completely positive form, and we conclude that the evolution is given by a completely positive map.

5.6 Conclusions to this chapter

In this chapter, we discussed the evolution of open systems and show two examples of when the evolution is given by a non completely positive map. In one example, the open system is initially entangled, and in the second example the open system is initially in a separable, but not simply separable, state.

We show that the non completely positive maps can be explained by defining an extension map, that relates the state of the open system to the overall state. The non completely positive maps are therefore a consequence of how the problem

is setup, rather than a consequence of a physical process. The evolution is only physically defined on the compatibility domain of states, even though the map is mathematically (linearly) defined on all states.

Finally we find that the map describing the evolution of an open system is not necessarily non-positive when the system is not simply separable, an open system that is initially in a zero discord form will have an evolution that is given by a completely positive map.

Chapter 6

Process tomography of open systems

Some experiments [51] in quantum process tomography have found negative maps in their results. Do these negative maps occur for the same reasons as discussed in the last chapter? As we will show, it is a closely related problem, and it leads to a more serious systemic problem with the theory of quantum process tomography as applied to open systems. We will begin by reviewing the fundamentals of quantum process tomography [50], and then move on to our results on bi-linear quantum process tomography and issues of quantum state preparation in experiments (to be published).

6.1 Introduction to Quantum process tomography

In quantum process tomography [50], the objective is to determine the action of a quantum process. We will think of the quantum process as a black box. We wish to determine what happens inside this black box, therefore we will feed different

quantum states as inputs to the black box and see what comes out; for each input state, we will measure the corresponding output state. If we know what the output state will be for any input state, then the behavior of this process is determined.

$$\text{Input states} \rightarrow \text{PROCESS} \rightarrow \text{Output states} \tag{6.1}$$

Assuming the quantum process can be described by a linear dynamical map, we need only pick a finite number of input states for our experiment. These input states should fully span the space of density matrices. Once we know how these states evolve, then by linearity we know how any input state will evolve. For example, for 2-level qubits, the following density matrices form a linearly independent and complete set of matrices:

$$\begin{aligned} P^{(1)} &= 1 + \sigma_x \\ P^{(2)} &= 1 - \sigma_x \\ P^{(3)} &= 1 + \sigma_y \\ P^{(4)} &= 1 + \sigma_z \end{aligned} \tag{6.2}$$

If we know the output states corresponding to each of these input states, then the map describing the quantum process can be determined. We note that to fully measure the density matrix of the output states, we will need to employ quantum state tomography (to be differentiated from process tomography), which adds another level of experimental complexity, but nonetheless is straightforward and is still experimentally practical.

Suppose each of these input states $P^{(i)}$ evolve to corresponding output state $Q^{(i)}$. We can write the map for the quantum process in terms of $P^{(i)}$ and $Q^{(i)}$, in its A-matrix form, as follows:

$$\mathcal{A}_{rs,r's'} = \sum_i Q_{rs}^{(i)} \tilde{P}_{r's'}^{(i)} \tag{6.3}$$

where $\tilde{P}^{(i)}$ is the dual satisfying:

$$\sum_{rs} \tilde{P}_{rs}^{(i)} P_{rs}^{(j)} = \delta_{ij} \tag{6.4}$$

We can easily verify that:

$$\left[\mathcal{A}\left(P^{(i)}\right)\right]_{rs} = \sum_j Q_{rs}^{(j)} \sum_{r's'} \tilde{P}_{r's'}^{(j)} P_{r's'}^{(i)} = Q_{rs}^{(i)} \tag{6.5}$$

6.2 A basic problem in Quantum process tomography

It is easy for theorists to require that a set of specific input states be used for process tomography. However, for a real world experiment, preparing these input states is not a trivial task. As we will see in this section, how the input states are prepared, when dealing with open systems, can fundamentally alter the results from quantum process tomography.

A quantum process tomography experiment may be broken down into basic stages. In the initial stage, just before the experiment begins, the system and environment is in a state pre-determined by the universe, but unknown to the experimenter. In the preparation stage, the experimenter attempts to prepare the system into a known input state for the experiment. In the evolution stage, the system and environment is allowed to evolve in time, through the process that we are trying to determine. In the final measurement stage, the output state from the process is measured and determined.

$$\begin{aligned}&\text{Unknown initial state} \rightarrow \text{Preparation into input state}\\ &\rightarrow \text{PROCESS} \rightarrow \text{Output state measured}\end{aligned} \tag{6.6}$$

Let us write the initial state, before the experiment begins ($t = 0_-$), of the system and environment as γ_0. This state is pre-determined by the universe and is unknown at this time to the experimenter. The experimenter only has access to the system and not the environment, so measurements can only be made to the system.

Starting in an unknown state is clearly undesirable to any experiment. Therefore, at the start of the experiment ($t = 0$), the experimenter will seek to prepare the system into a known initial state. The simplest method is to make a measurement. Let us assume the measurement is given by the von Neumann model, with a set of orthonormal projections $P^{(n)}$, where $1 \leq n \leq N$ is the index marking the nth projection of the set.

After the measurement, suppose the nth outcome is detected, the global (system and environment) state is then given by:

$$\gamma(t = 0; n) = \frac{1}{\Gamma_n} P^{(n)} \gamma_0 P^{(n)} \tag{6.7}$$

where $\Gamma^{(n)} = Tr[P^{(n)}\gamma_0]$ is the normalization for this state, and also represents the probability of obtaining the nth outcome.

The expectation state of the system and environment after the measurement, at the start of the experiment, is given by:

$$\gamma(t = 0) = \sum_n P^{(n)} \gamma_0 P^{(n)} \tag{6.8}$$

We note that the state of the system and environment has been modified by the action of the measurement. The original state could be written as:

$$\gamma_0 = \sum_{nm} P^{(n)} \gamma_0 P^{(m)} \tag{6.9}$$

The state of the system and environment collapses after the measurement, which destroys the cross terms for $n \neq m$.

We can also write the state for the system and environment following the measurement as:

$$\gamma(t=0) = \sum_{n} \Gamma^{(n)} P^{(n)} \otimes \tau^{(n)} \tag{6.10}$$

where $\tau^{(n)} = \frac{1}{\Gamma^{(n)}} Tr_{\mathbb{A}}[P^{(n)} \gamma_0]$ is the normalized environment state associated with outcome n. This is a zero discord state as discussed in previous chapters. We should distinguish this from a simply separable state of the form:

$$\left(\sum_{n} \Gamma^{(n)} P^{(n)} \right) \otimes \tau \tag{6.11}$$

Ideally we would prefer to have the simply separable state following the preparation stage of the experiment. A simply separable state is not correlated to the environment, since the state of the environment is independent of n. On the other hand, a zero discord state remains correlated to the environment, since the environment state depends on the outcome n. This subtle difference is key to the problem, as we will soon show, the dependence of the environment state on the outcome is what leads to a non-linear evolution.

In the next stage of the experiment, the system and environment are allowed to evolve for time T. If the nth outcome was recorded in the preparation stage, the evolution is given by:

$$\begin{aligned}\gamma(t=T;n) &= U\gamma(t=0;n)U^{\dagger} \\ &= \tfrac{1}{\Gamma^{(n)}} U P^{(n)} \gamma_0 P^{(n)} U^{\dagger}\end{aligned} \tag{6.12}$$

Finally the system is measured, using a state tomography process, and we can determine the output density matrix $Q^{(n)}$, which is given by the 'process equation':

$$\begin{aligned}Q^{(n)} &= Tr_{\mathbb{B}}[\gamma(t=T;n)] \\ &= \tfrac{1}{\Gamma^{(n)}} Tr_{\mathbb{B}}[U P^{(n)} \gamma_0 P^{(n)} U^{\dagger}]\end{aligned} \tag{6.13}$$

Let us expand this process equation with matrix indices:

$$\begin{aligned}Q^{(n)}_{r,s} &= \tfrac{1}{\Gamma^{(n)}} U_{r\epsilon,r'\alpha} P^{(n)}_{r',r''} \gamma_{0 r''\alpha,s''\beta} P^{(n)}_{s'',s'} U^{*}_{s\epsilon,s'\beta} \\ &= \tfrac{1}{\Gamma^{(n)}} P^{(n)}_{r'r''} M^{(r,s)}_{r'r'',s's''} P^{(n)}_{s's''}\end{aligned} \tag{6.14}$$

where we define the matrix M as (note that the superscript indices match the elements on the LHS of the equation, while the subscript indices match elements on the RHS of the equation):

$$M^{(r,s)}_{r'r'',s's''} = \sum_{\alpha\beta\epsilon} U_{r\epsilon,r'\alpha} \gamma_{0 r''\alpha,s''\beta} U^{*}_{s\epsilon,s'\beta} \tag{6.15}$$

Is this process a linear map? The process is a linear map on the initial state γ_0. However it is bi-linear on the states $P^{(n)}$, which we consider to be the input states to the quantum process.

In standard Quantum process tomography, we assume the states $P^{(n)}$ are the initial states of the process. For the purpose of tomography, the unknown state γ_0 is not of interest to us. But the above equation tells us that we cannot describe the process as a linear map of the states $P^{(n)}$.

The process has a bi-linear dependence on $P^{(n)}$ because the environment

state depends on the state of the system. If we write the process equation 6.13 as:

$$Q^{(n)} = Tr_{\mathbb{B}}[UP^{(n)} \otimes \tau^{(n)}U^{\dagger}] \tag{6.16}$$

and since

$$\tau^{(n)} = \frac{1}{\Gamma^{(n)}} Tr_{\mathbb{B}}[\gamma_0 P^{(n)}] \tag{6.17}$$

then we can clearly see that the environment state $\tau^{(n)}$ is in effect a function of $P^{(n)}$. This correlation between the environment and the system causes the non-linearity in the process.

6.3 Quantum Process Tomography for open systems

We now know that the evolution of the input state $P^{(n)}$ through the quantum process under investigation, is given by the matrix M, acting bi-linearly on the state $P^{(n)}$. Therefore, the matrix M fully describes the process; given M, we can determine the output state of any input state we can prepare by measurement. Our objective then is to determine the matrix M.

Let us consider the results available to the experimenter at this point. The projections $P^{(n)}$ are predetermined by the experimenter. If the experiment is repeated enough times, $Q^{(n)}$ and $\Gamma^{(n)}$ can be measured. Therefore the known quantities are $P^{(n)}$, $Q^{(n)}$ and $\Gamma^{(n)}$.

We can interpret the process equation 6.14 in a simpler form as follows:

$$\langle P^{(n)}|M|P^{(n)}\rangle = \Gamma^{(n)}Q^{(n)} \tag{6.18}$$

In this form, we will consider M to be a $N^2 \times N^2$ matrix of elements, each element is a $N \times N$ matrix. As in the case with linear maps, this matrix M is hermitian, the transpose of M gives the conjugate element (the adjoint matrix):

$$\begin{aligned} M^{(r,s)}_{r'r'',s's''} &= \textstyle\sum_{\alpha\beta\epsilon} U_{r\epsilon,r'\alpha}\gamma_{0r''\alpha,s''\beta}U^{\dagger}_{s'\beta,s\epsilon} \\ &= \textstyle\sum_{\alpha\beta\epsilon} U^{T}_{r'\alpha,r\epsilon}\gamma_{0s''\beta,r''\alpha}^{*}U^{*}_{s\epsilon,s'\beta} \\ &= {M^{(s,r)}_{s's'',r'r''}}^{*} \end{aligned} \tag{6.19}$$

The trace of M gives an element with unit trace:

$$\begin{aligned} \textstyle\sum_{rr'r''} M^{(r,r)}_{r'r'',r'r''} &= \textstyle\sum_{rr'r''\alpha\beta\epsilon} U_{r\epsilon,r'\alpha}\gamma_{0r''\alpha,r''\beta}U^{\dagger}_{r'\beta,r\epsilon} \\ &= \textstyle\sum_{r''\alpha\beta} \delta_{\alpha\beta}\gamma_{0r''\alpha,r''\beta} \\ &= 1 \end{aligned} \tag{6.20}$$

Given these properties, M would have $\frac{1}{2}(N^4 + N^2)$ elements. Therefore we would need $\frac{1}{2}(N^4 + N^2)$ independent equations of the form 6.18 to fully determine M. Fortunately, as we will show, we will not need to fully determine M.

Let us proceed by considering a 2-level (qubit) system, the simplest quantum system. Now consider our process equation $\langle P^{(n)}|M|P^{(n)}\rangle = \Gamma^{(n)}Q^{(n)}$. In this form, we wish to consider $P^{(n)}$ as a vector. Fortunately, there already exists an easy way to write $P^{(n)}$ as a vector. For a 2-level system, the projections $P^{(n)}$ can be written as:

$$P^{(n)} = \frac{1}{2}(I + p^{(n)}_1\sigma_1 + p^{(n)}_2\sigma_2 + p^{(n)}_3\sigma_3) \tag{6.21}$$

where σ_1, σ_2 and σ_3 are the Pauli matrices, and the coefficients $p^{(n)}_i$ are real. For a projection of a 2-level system, the coefficients must satisfy $\sum_i (p^{(n)}_i)^2 = 1$.

The matrices I and σ_i together forms a vector basis for this space. Therefore

equation 6.21 is simply a vector decomposition of $P^{(n)}$ in a fixed basis. Our process equation can be expanded as:

$$\langle I|M|I\rangle + p_i^{(n)}\langle I|M|\sigma_i\rangle + p_i^{(n)}\langle \sigma_i|M|I\rangle + p_i^{(n)}p_j^{(n)}\langle \sigma_i|M|\sigma_j\rangle = 4\Gamma^{(n)}Q^{(n)} \tag{6.22}$$

Let us consider some specific projections. For the projection $\frac{1}{2}(I+\sigma_1)$, we have:

$$\langle I+\sigma_1|M|I+\sigma_1\rangle = \langle I|M|I\rangle + \langle I|M|\sigma_1\rangle + \langle \sigma_1|M|I\rangle + \langle \sigma_1|M|\sigma_1\rangle \tag{6.23}$$

Similarly for the projection $\frac{1}{2}(I-\sigma_1)$:

$$\langle I-\sigma_1|M|I-\sigma_1\rangle = \langle I|M|I\rangle - \langle I|M|\sigma_1\rangle - \langle \sigma_1|M|I\rangle + \langle \sigma_1|M|\sigma_1\rangle \tag{6.24}$$

The two equations above can be solved simultaneously to give us the following unknowns:

$$\begin{aligned} &\langle I|M|I\rangle + \langle \sigma_1|M|\sigma_1\rangle \\ &\langle I|M|\sigma_1\rangle + \langle \sigma_1|M|I\rangle \end{aligned} \tag{6.25}$$

Similarly if we repeat the exercise for the σ_2 and σ_3 basis, we can find the following:

$$\begin{aligned} &\langle I|M|I\rangle + \langle \sigma_i|M|\sigma_i\rangle \\ &\langle I|M|\sigma_i\rangle + \langle \sigma_i|M|I\rangle \end{aligned} \tag{6.26}$$

To obtain the cross terms $\langle\sigma_i|M|\sigma_j\rangle$, we can use projections such as $\frac{1}{2}(I + \frac{1}{\sqrt{2}}\sigma_1 + \frac{1}{\sqrt{2}}\sigma_2)$, which gives:

$$\begin{aligned}
&\langle I|M|I\rangle + \tfrac{1}{2}\langle\sigma_1|M|\sigma_1\rangle + \tfrac{1}{2}\langle\sigma_2|M|\sigma_2\rangle \\
&+\tfrac{1}{\sqrt{2}}\langle I|M|\sigma_1\rangle + \tfrac{1}{\sqrt{2}}\langle\sigma_1|M|I\rangle \\
&+\tfrac{1}{\sqrt{2}}\langle I|M|\sigma_2\rangle + \tfrac{1}{\sqrt{2}}\langle\sigma_2|M|I\rangle \\
&+\tfrac{1}{2}\langle\sigma_1|M|\sigma_2\rangle + \tfrac{1}{2}\langle\sigma_2|M|\sigma_1\rangle
\end{aligned} \tag{6.27}$$

Eliminating the terms found previously, this gives us the cross term:

$$\frac{1}{2}\langle\sigma_1|M|\sigma_2\rangle + \frac{1}{2}\langle\sigma_2|M|\sigma_1\rangle \tag{6.28}$$

So to summarize, we use the following nine projections:

$$\begin{aligned}
&\tfrac{1}{2}(I + \sigma_i) \\
&\tfrac{1}{2}(I - \sigma_i) \\
&\tfrac{1}{2}(I + \tfrac{1}{\sqrt{2}}\sigma_1 + \tfrac{1}{\sqrt{2}}\sigma_2) \\
&\tfrac{1}{2}(I + \tfrac{1}{\sqrt{2}}\sigma_1 + \tfrac{1}{\sqrt{2}}\sigma_3) \\
&\tfrac{1}{2}(I + \tfrac{1}{\sqrt{2}}\sigma_2 + \tfrac{1}{\sqrt{2}}\sigma_3)
\end{aligned} \tag{6.29}$$

Solving the simultaneous equations we can obtain the following matrix elements:

$$\begin{aligned}
&\langle I|M|I\rangle + \langle\sigma_i|M|\sigma_i\rangle \\
&\langle I|M|\sigma_i\rangle + \langle\sigma_i|M|I\rangle \\
&\langle\sigma_i|M|\sigma_j\rangle + \langle\sigma_j|M|\sigma_i\rangle
\end{aligned} \tag{6.30}$$

One might point out that this is not enough to fully determine M. However we notice that the elements we found are sufficient to determine the output state for any projection $P^{(n)}$, since we can re-write equation 6.22 as:

$$
\begin{aligned}
&\textstyle\sum_i (p_i^{(n)})^2 \left(\langle I|M|I\rangle + \langle \sigma_i|M|\sigma_i\rangle\right) \\
&+ \textstyle\sum_i p_i^{(n)} \left(\langle I|M|\sigma_i\rangle + \langle \sigma_i|M|I\rangle\right) \\
&+ \textstyle\sum_{j>i} p_i^{(n)} p_j^{(n)} \left(\langle \sigma_i|M|\sigma_j\rangle + \langle \sigma_j|M|\sigma_i\rangle\right) \\
&= 4\Gamma^{(n)} Q^{(n)}
\end{aligned}
\tag{6.31}
$$

where we used the property $\sum_i (p_i^{(n)})^2 = 1$. We can make some observations here: we see that only the sums of the cross terms $\langle \sigma_i|M|\sigma_j\rangle + \langle \sigma_j|M|\sigma_i\rangle$ can appear, because the coefficients $p_i^{(n)}$ are real. We also see that the element $\langle I|M|I\rangle$ is always paired with a diagonal element $\langle \sigma_i|M|\sigma_i\rangle$ as long as the state is a pure projection satisfying $\sum_i (p_i^{(n)})^2 = 1$. The diagonal element $\langle I|M|I\rangle$ only has to be known if the system can be prepared directly to a mixed state such that $\sum_i {p_i^{(n)}}^2 < 1$. This may be accomplished by a generalized measurement. If we allow generalized measurement, then we need just one more input state, for example we can choose $\frac{1}{2}I + \frac{1}{4}\sigma_1$, which gives us another independent equation that can be solved to obtain $\langle I|M|I\rangle$.

Therefore we conclude that the elements of M found in 6.31 are all that are needed to describe the process. We now have a correct Quantum Process Tomography procedure for an open 2-level system.

The generalization to N-level systems remains to be done. We can use the generalized Pauli/Gellman hermitian traceless $N \times N$ matrices [53] to decompose any density matrix, so the decomposition only has real coefficients. Unfortunately the coefficients no longer satisfy just the simple equation $\sum_i (p_i^{(n)})^2 = 1$. The additional constraints on the coefficients complicate the task of constructing the projections needed to span the matrix elements of M.

6.4 Other possible Quantum Process Tomography procedures

One might question if the above procedure is the only viable process tomography procedure for an open system. We will address two possible alternative procedures in this section and the next section.

If our objective is to determine this interaction transformation U that acts on our system and environment, then perhaps it is not necessary to prepare our system into different states. Implicitly our tomography procedure requires a large number of similar systems, since we have to repeat our experiment with many particles in order to measure the parameters we need. Given many similar systems, perhaps we can simply divide them into two groups. We can take one group and perform state tomography immediately, in order to determine the initial state of the system. The other group is left alone until the end of the experiment, where we perform state tomography to determine the final state of the system.

The process equation may then be written as:

$$Q = Tr_{\mathbb{B}}[U\gamma_0 U^\dagger] = \Lambda(\rho) \tag{6.32}$$

where $\rho = Tr_{\mathbb{B}}[\gamma_0]$ is known when we perform state tomography at the start of the experiment on half the available samples. Q is known when we perform state tomography at the end of the experiment, on the other half of the samples.

However we can see that this is not a tomography procedure. We only know one initial state and one final state, this is clearly insufficient to fully, or even substantially, determine the linear map Λ.

Therefore it is clear that to perform process tomography, we need to perform

some sort of preparation of the system into a variety of states, in order to determine how the process evolves these states. In the next section, we propose a different tomography procedure, with the objective of decoupling the environment from the system. If the environment is not correlated with the system, then the bi-linear terms would not exist, and linear process tomography can be applied.

6.5 Stochastic preparation for process tomography

One way to decouple the environment from the system is to use a pin map. Consider a pin map Λ, which takes any density matrix ρ to a fixed pure state $|\Phi\rangle$:

$$\Lambda(\rho) = |\Phi\rangle\langle\Phi| \tag{6.33}$$

If we apply this to our open system, we get:

$$\Lambda \otimes I\left(\gamma_0\right) = |\Phi\rangle\langle\Phi| \otimes \tau \tag{6.34}$$

where $\tau = Tr_{\mathbb{A}}[\gamma_0]$. By fixing the system into a single state, the pin map effectively destroys any correlations that exist between the system and environment.

If we can legitimately consider such stochastic processes for open systems, then a different possibility for a tomography procedure exists. A pin map is applied at the start of the experiment, to eliminate any correlations between the system and environment. Once the system has been decoupled from the environment, the experimenter can then proceed to prepare the input states, which we can write in general as stochastic maps:

$$\Omega^{(n)}\left(|\Phi\rangle\langle\Phi|\right) = P^{(n)} \tag{6.35}$$

The overall process then can be summarized by this equation:

$$\begin{aligned} Q^{(n)} &= Tr_{\mathbb{B}}[U(\Omega^{(n)} \circ \Lambda) \otimes I(\gamma_0) U^\dagger] \\ &= Tr_{\mathbb{B}}[UP^{(n)} \otimes \tau U^\dagger] \end{aligned} \tag{6.36}$$

This process equation is linear on $P^{(n)}$. Therefore the map describing this process is linear.

While these stochastic maps are legitimate in theory, one may ask how this can be performed experimentally. For the pin map, perhaps the simplest scenario is for the experimenter to make a von Neumann measurement on the system, then rotate the system accordingly (unitary transformation) based on the outcome he records. So for example, working with a qubit, a measurement is made in the σ_x basis. If the $+x$ state is observed, the system is left alone. If the $-x$ state is observed, then the experimenter flips a switch to rotate the system to the $+x$ state. This performs a pin map to the $+x$ state.

However we should consider whether the measurement and rotation apparatus, or even the experimenter, is part of the quantum environment. If they are part of the quantum environment, then are stochastic maps, or even von Neumann measurements, legitimately possible?

We know from earlier chapters that the set of stochastic maps $\Omega^{(n)} \circ \Lambda = \Pi^{(n)}$, is nothing more than a generalized measurement. Assuming an equal number of each input state is prepared, the overall map is:

$$\Pi = \frac{1}{K} \sum_{n=1}^{K} \Pi^{(n)} \tag{6.37}$$

This generalized measurement can be performed by a unitary transformation and von Neumann measurement by introducing a suitable ancillary system. If these

ancillary systems are part of the environment, then perhaps the true process is still of a bi-linear form?

Let us investigate this problem in more detail. Suppose we use an ancillary system $\mathbb{C}$ to perform the generalized measurement. The ancillary system is initialized to the state $\epsilon^{\mathbb{C}}$. The generalized measurement is implemented with a unitary transformation V and von Neumann measurement, where the map $\Pi^{(n)}$ is associated with the projection $J^{(n)}$ of the measurement:

$$\Pi^{(n)}(\rho^{\mathbb{A}}) = Tr_{\mathbb{C}}[{J^{(n)}}^{\mathbb{C}} V^{\mathbb{A}\mathbb{C}} \rho^{\mathbb{A}} \otimes \epsilon^{\mathbb{C}} {V^{\mathbb{A}\mathbb{C}}}^{\dagger} {J^{(n)}}^{\mathbb{C}}] \tag{6.38}$$

Note that we have carefully denoted the primary system $\mathbb{A}$ and ancillary $\mathbb{C}$. Now let us take this and include it within the overall problem including the environment $\mathbb{B}$, to get the overall process equation:

$$Q^{(n)^{\mathbb{A}}} = Tr_{\mathbb{B}\mathbb{C}}[U {J^{(n)}}^{\mathbb{C}} V^{\mathbb{A}\mathbb{C}} \gamma_0^{\mathbb{A}\mathbb{B}} \otimes \tau_0^{\mathbb{C}} {V^{\mathbb{A}\mathbb{C}}}^{\dagger} {J^{(n)}}^{\mathbb{C}} U^{\dagger}] \tag{6.39}$$

If U acts only on $\mathbb{A}$ and $\mathbb{B}$, and not on $\mathbb{C}$, then we can simplify:

$$\begin{aligned} Q^{(n)^{\mathbb{A}}} &= Tr_{\mathbb{B}}\left[U Tr_{\mathbb{C}}[{J^{(n)}}^{\mathbb{C}} V^{\mathbb{A}\mathbb{C}} \gamma_0^{\mathbb{A}\mathbb{B}} \otimes \tau_0^{\mathbb{C}} {V^{\mathbb{A}\mathbb{C}}}^{\dagger} {J^{(n)}}^{\mathbb{C}}] U^{\dagger}\right] \\ &= Tr_{\mathbb{B}}[U \Pi^{(n)^{\mathbb{A}}} \otimes I^{\mathbb{B}} \left(\gamma_0^{\mathbb{A}\mathbb{B}}\right) U^{\dagger}] \\ &= Tr_{\mathbb{B}}[U P^{(n)^{\mathbb{A}}} \otimes \tau^{\mathbb{B}} U^{\dagger}] \end{aligned} \tag{6.40}$$

Therefore we get a linear map if U does not act on the ancillary system $\mathbb{C}$.

One may bring up a subtle issue, that is the preparation of the ancillary $\mathbb{C}$ into the state $\epsilon^{\mathbb{C}}$. We must assume that any additional systems used to prepare the ancillary system is also completely isolated from the primary system $\mathbb{A}$.

We can conclude that for the purpose of the experiment, any system that does not otherwise interact with the primary system $\mathbb{A}$ from $0 < t < T$ need not

be included in the environment $\mathbb{B}$. On the other hand if an ancillary system is not perfectly isolated from the system during the experiment, then the ancillary system is part of the environment, and we cannot assume the process is represented by as a linear map.

Fortunately it should be possible to verify if a process is given by a bi-linear map or a linear map, since the two different maps give very different predictions. We will develop such a verification procedure in the following section.

6.6 Bi-linear vs. linear map verification procedure

The bi-linear map M we have considered in this chapter is incompatible with the behavior of a linear map. Consider what happens to a state that is a linear combination of a set of projections:

$$X = \sum_n c_n P^{(n)} \tag{6.41}$$

If the bi-linear map is compatible in some way with a linear process, then we would be able to write:

$$\langle X|M|X\rangle = \sum_n c_n \langle P^{(n)}|M|P^{(n)}\rangle \tag{6.42}$$

Expanding the LHS gives us:

$$\sum_{mn} c_m^* c_n \langle P^{(m)}|M|P^{(n)}\rangle = \sum_n c_n \langle P^{(n)}|M|P^{(n)}\rangle \tag{6.43}$$

It is clear that no non-trivial conditions can exist for M that will allow this equality for arbitrary coefficients c_n.

Therefore the bi-linear map gives different predictions from a linear map. In that case, we should be able to distinguish between whether a process is given by a linear map or a bi-linear map. Let us consider the example of the tomography procedure we had proposed for a 2-level system.

In our procedure, we suggested the following input states:

$$\begin{aligned}
P^{(1)} &= \tfrac{1}{2}(I+\sigma_1) \\
P^{(2)} &= \tfrac{1}{2}(I-\sigma_1) \\
P^{(3)} &= \tfrac{1}{2}(I+\sigma_2) \\
P^{(4)} &= \tfrac{1}{2}(I-\sigma_2) \\
P^{(5)} &= \tfrac{1}{2}(I+\sigma_3) \\
P^{(6)} &= \tfrac{1}{2}(I-\sigma_3) \\
P^{(7)} &= \tfrac{1}{2}(I+\tfrac{1}{\sqrt{2}}\sigma_1+\tfrac{1}{\sqrt{2}}\sigma_2) \\
P^{(8)} &= \tfrac{1}{2}(I+\tfrac{1}{\sqrt{2}}\sigma_1+\tfrac{1}{\sqrt{2}}\sigma_3) \\
P^{(9)} &= \tfrac{1}{2}(I+\tfrac{1}{\sqrt{2}}\sigma_2+\tfrac{1}{\sqrt{2}}\sigma_3)
\end{aligned} \tag{6.44}$$

If our process is given by a linear map, then these 9 input states is over complete, we would only have needed 4 input states to determine a linear map. This discrepancy is summarized by the following linear sum rules:

$$P^{(1)} + P^{(2)} = P^{(3)} + P^{(4)} = P^{(5)} + P^{(6)} \tag{6.45}$$

$$P^{(7)} = (\frac{1}{2} - \frac{1}{\sqrt{2}})(P^{(1)} + P^{(2)}) + \frac{1}{\sqrt{2}}(P^{(1)} + P^{(3)}) \tag{6.46}$$

$$P^{(8)} = (\frac{1}{2} - \frac{1}{\sqrt{2}})(P^{(1)} + P^{(2)}) + \frac{1}{\sqrt{2}}(P^{(1)} + P^{(5)}) \tag{6.47}$$

$$P^{(9)} = (\frac{1}{2} - \frac{1}{\sqrt{2}})(P^{(1)} + P^{(2)}) + \frac{1}{\sqrt{2}}(P^{(3)} + P^{(5)}) \tag{6.48}$$

If the process is linear, then the output states must satisfy the same sum rules, which we obtain from the above equations by suitably writing Q in place of P. If these sum rules are not satisfied, then the process is not linear. However satisfying the sum rules is only necessary but not sufficient to determine if the process is linear; a bi-linear map can still be constructed from this set of input and output states without contradiction. Therefore an additional input state, distinct from the above nine input states, should be tested to determine which side of equation 6.43 is satisfied. More explicitly, if we introduce an additional input state:

$$X = \sum_n c_n P^{(n)} \tag{6.49}$$

and the corresponding output state is found to be $\sum_n c_n Q^{(n)}$, then the process is linear. However if the corresponding output state is given by $\sum_{mn} c_m^* c_n \langle P^{(m)}|M|P^{(n)}\rangle$ then the process is bi-linear.

6.7 Fundamental questions on preparation and measurements

The above problems, regardless of the subject of process tomography, poses some interesting fundamental questions about preparing quantum states for experiments.

We realize that at the beginning of any experiment, the quantum system or particle would exist in an unknown state that could be (and most likely is) entangled with an environment. Preparation of the system or particle into a known state is a necessary part of any experiment. Therefore, it is clear that some care has to be taken to ensure that the preparation apparatus, the ancillary systems employed to perform stochastic maps or generalized measurements, remains isolated from the

system for the duration of the experiment, except during specific events.

If interaction occurs between the system and this environment, then non-linear noise can be introduced into the experiment. Quantum error correction protocols proposed so far are based on correcting linear noise. If bi-linear errors occur, error correction becomes a more difficult challenge.

We propose that the verification procedure given in the last section can be used to confirm the proper isolation of the apparatus and ancillary systems during an experiment.

A related problem is the state collapse during the von Neumann measurement on an open system. We stated that the state collapses in the following way:

$$\gamma_0 \rightarrow (P^{(n)} \otimes I)\gamma_0(P^{(n)} \otimes I) \tag{6.50}$$

This collapse of the quantum state is not a linear process, and is what leads us to the bi-linear map M. Without the collapse of the state during the preparation, there will be no bi-linear terms, and the process would be linear. Therefore, the tomography procedure from the last section can also be used to check a physical implementation of a von Neumann measurement.

6.8 Analysis of a Quantum Process Tomography experiment

With everything we now know, let us analyze a quantum process tomography experiment performed by M. Howard et. al [51].

In this experiment, the system that is studied is an electron configuration formed in a nitrogen vacancy defect in a diamond lattice. The quantum state of the

system is given by a spin triplet (S=1). Again we will write the initial state of the system and environment as γ_0.

The system is prepared by optical pumping, which results in a strong spin polarization. The state of the system is said to have 70% chance of being in a pure state $|\phi\rangle$. Or more mathematically, we would write that the probability $Tr[|\phi\rangle\langle\phi|\gamma_0] = 0.7$.

Since the population probability is high, an assumption was made that the state of the system can be simply approximated as a pure state $|\phi\rangle\langle\phi|$. From this initial state, different input states can be prepared by suitably applying microwave pulses resonant with the transition levels. After preparation, the system is allowed to evolve, and the final states (density matrices) are measured. With the knowledge of the initial state and the measured final states, the linear map that should describe this process is determined.

It was found that the map has negative eigenvalues, so the map was "corrected" using a least squares fit between the experimentally determined map and a theoretical map based on Hermitian parametrization [52], while enforcing complete positivity.

However, if we do not regard the negative eigenvalues of the map as aberrations, then we should consider the assumptions about the preparation of the system more carefully. The assumption about the initial state of the system is:

$$\gamma_0 \rightarrow |\phi\rangle\langle\phi| \otimes \tau \tag{6.51}$$

This is in effect a pin map. Together with the stochastic transformation of the initial state into the various input states, this is identical to the stochastic preparation method that we discussed.

It is clear that the pure initial state assumption is unreasonable, given our knowledge now of how the process is sensitive to initial correlations between the system and the environment. If we discard that assumption, then we would write the process equation as:

$$Q^{(n)} = Tr_{\mathbb{B}}[U\Pi^{(n)} \otimes I(\gamma_0)U^{\dagger}] \tag{6.52}$$

where $\Pi^{(n)}$ is the stochastic mapping corresponding to preparing the nth input state. We will assume that the stochastic process does not involve any ancillary systems that interact with the primary system during the experiment.

In this experiment, $\Pi^{(n)}$ is nothing more than a unitary transformation $V^{(n)}$ satisfying $V^{(n)}|\phi\rangle = |\phi^{(n)}\rangle$, where $|\phi^{(n)}\rangle$ is the desired pure nth input state to the process.

We can write $V^{(n)} = |\phi^{(n)}\rangle\langle\phi| + \ldots$ and write the equation as:

$$Q^{(n)} = Tr_{\mathbb{B}}[U|\phi^{(n)}\rangle\langle\phi|\gamma_0|\phi\rangle\langle\phi^{(n)}|U^{\dagger}] + \ldots \tag{6.53}$$

Therefore, to first approximation, since $\langle\phi|\gamma_0|\phi\rangle = 0.7$, the process is a linear mapping on the states $|\phi^{(n)}\rangle\langle\phi^{(n)}|$. However it is clear that if we include all terms, the process is not truly a linear map on the states $|\phi^{(n)}\rangle\langle\phi^{(n)}|$. The negative eigenvalues are therefore a result of fitting results into a linear map matrix when the process is not truly represented by a linear map matrix.

6.9 Conclusions to this chapter

There are some subtle but fundamental issues on the issue of state preparation in experiments, that has not been discussed much in theory. We presented two main

theoretical methods for preparing quantum systems for experiments, the measurement preparation method or the stochastic preparation method. We find that in both cases, the system is set initially into a separable state with the environment. However, the two methods give very different outcomes.

With the measurement method, the initial state is not simply separable, and consequently contains correlations with the environment. The evolution of such a system is given by a bi-linear map. The determination of this bi-linear map by process tomography is more difficult, but we developed a procedure that works for qubit systems.

With the stochastic method, the initial state can be made simply separable, effectively de-coupling the system from the environment. The evolution of the system is then given by a linear map. However we find that the isolation of the apparatus from the system during the experiment is of greater importance with this method. Any apparatus or ancillary systems used for the stochastic preparation must not be contained in the quantum environment, the quantum environment being defined as everything that interacts with the quantum system during the experiment.

We discussed a verification protocol that can be used to distinguish bi-linear processes from linear processes. This protocol may become an important tool in experiments, as it can confirm that the apparatus used for measurements and stochastic procedures is properly isolated from the quantum system during the experiment.

Bibliography

[1] A. Kuah and E.C.G. Sudarshan, *Dynamical maps and measurements*, arXiv:quant-ph/0209083

[2] A. Kuah and E.C.G. Sudarshan, *Manifold of density matrices*, arXiv:quant-ph/0307218

[3] A. Kuah and E.C.G. Sudarshan, *Extension maps*, arXiv:quant-ph/0503119

[4] A. Kuah and E.C.G. Sudarshan, *Schmidt states and positivity of linear maps*, arXiv:quant-ph/0506095

[5] C.A. Rodriguez, K. Modi, A. Kuah, E.C.G. Sudarshan and A. Shaji, *Completely Positive Maps and Classical Correlations*, arXiv:quant-ph/0703022

[6] J. von Neumann, Gott. Nach. (1927) 157, 245 272

[7] J.Preskill, *Lecture Note for Physics: Quantum Information and Computation*, http://theory.caltech.edu/people/preskill

[8] A. Einstein, B. Podolsky and N. Rosen, Phys. Rev. 47 (1935) 777

[9] E. Schrodinger, Naturwissenchaften 23 (1935) 807

[10] J. von Neumann, Mathematische Grundlagen der Quantenmechanik (Springer, Berlin) 1932

[11] J.S. Bell, Physics 1 (1964) 195

[12] J.M. Jauch and C. Piron, Helv. Phys. Acta 40 (1967) 559

[13] E.B. Davies and J.T. Lewis, Comm. Math. Phys. 17 (1970)

[14] W.F. Stinespring, *Positive functions on C*-algebras*, Proceedings of the American Mathematical Society (1955) 211-216

[15] E.C.G. Sudarshan, P.M. Mathews, and J. Rau, *Stochastic Dynamics of Quantum-Mechanical Systems*, The Physical Review 121 (1961) 920-924

[16] E.C.G. Sudarshan and T.F. Jordan, *Dynamical Mappings of Density Operators in Quantum Mechanics I*, Journal of Mathematical Physics Vol. 2 No. 6 (1961) 772-775

[17] E. Stormer, *Positive Linear Maps of Operator Algebras*, Acta Math. 110 (1963) 233

[18] M. Choi, *Positive Linear Maps on C*-Algebras* , Can. J. Math 24, 520-529 (1972)

[19] A. Jamiolkowski, *Linear transformations that preserve trace and positive semidefiniteness of operators*, Reports on Mathematical Physics Vol. 3 No. 4 (1972) 275-278

[20] G. Lindblad, Commun. Math. Phys. 40 (1975) 147

[21] S.L. Woronowicz, *Positive Maps of Low Dimensional Algebras*, Reports on Mathematical Physics 10 (1976) 165-183

[22] V. Gorini and E.C.G. Sudarshan, *Extreme Affine Transformations*, Comm. Math. Phys. 46 (1976) 43

[23] K. Kraus, *States, Effects and operations: Fundamental notions of Quantum Theory*, Lecture Notes in Physics 190 (1983)

[24] E.C.G. Sudarshan, *Quantum Measurement and Dynamical Maps*, From SU(3) to Gravity (Festschrift in honor of Yuval Ne'eman), E. Gotsman and G. Tauber (eds.), Cambridge University Press (1986) 433

[25] R.F. Werner, *Quantum states with Einstein-Podolsky-Rosen correlations admitting a hidden variable model*, Physical Review A Vol. 40 No. 8 (1989) 4277

[26] S. Popescu, Phys. Rev. Lett. 72 (1994) 797

[27] R. Horodecki and M. Horodecki, Phys. Rev. A 54 (1996) 1838

[28] M. Horodecki, P. Horodecki and R. Horodecki, *Separability of mixed states: necessary and sufficient conditions*, Physics Letters A 223 (1996) 1-8

[29] A. Peres, *Separability Criterion for Density Matrices*, Phys. Rev. Lett. 77 (1996) 1413

[30] M. Horodecki and P. Horodecki, *Reduction criterion of separability and limits for a class of protocols of entanglement distillation*, LANL preprint quant-ph/9708015

[31] M.S. Marinov, *Correction to invariant volumes of compact groups*, J. Phys. A: Math. Gen. 14 (1981) 543-544

[32] T. Tilma and E.C.G. Sudarshan, *Generalized Euler angle parametrization for SU(N)*, J. Phys. A: Math. Gen 35 (2002) 10467-10501

[33] E.C.G. Sudarshan and A. Shaji, *Structure and parametrization of stochastic maps of density matrices*, J. Phys. A 36 (2003) 5073-5081

[34] T.F. Jordan, A. Shaji and E.C.G. Sudarshan, *Dynamics of initially entangled open quantum systems*, Physical Review A 70 (2004) 1

[35] C.H. Bennett, D.P. DiVincenzo, J.A. Smolin and W.K. Wootters, *Mixed State Entanglement and Quantum Error Correcting Codes*, Phys. Rev. A 54 (1996) 3824

[36] C.H. Bennett, G. Brassard, S. Popescu, B. Schumacher, J.A. Smolin, and W.K. Wootters, *Purication of Noisy Entanglement and Faithful Teleportation via Noisy Channels*, Phys. Rev. Lett. 76 (1996) 722

[37] M. Hillery, Phys. Rev. A 35 (1987) 725

[38] M. Hillery, Phys. Rev. A 39 (1989) 2994

[39] D.J.C. Bures, Trans Am. Math. Soc. 135 (1969) 199

[40] A. Uhlmann, Rep. Math. Phys. 9 (1976) 273

[41] M. Hubner, Phys. Lett. A 163 (1992) 239

[42] A. Kuah and E.C.G. Sudarshan, *Extension maps*, LANL preprint quant-ph/0503119

[43] A. Ekert, Phys. Rev. Lett. 67 (1991) 661

[44] C.H. Bennett and S.J. Wiesner, Phys. Rev. Lett. 69 (1992) 2881

[45] C.H. Bennett, G. Brassard, C. Crepeau, R. Jozsa, A. Peres and W.K. Wootters, Phys. Rev. Lett. 70 (1993) 1895

[46] A. Barenco, D. Deutsch, A. Ekert and R. Jozsa, Phys. Rev. Lett. 74 (1995) 4083

[47] C.H. Bennett, D.P. Di Vincenzo, J. Smolin and W.K. Wootters, Phys. Rev. A 54 (1997) 3814

[48] H. Ollivier and W.H. Zurek, Phys. Rev. Lett. 88 (2001) 17901

[49] L. Henderson and V. Vedral, LANL preprint quant-ph/0105028 (2001)

[50] M.A. Nielsen and I.L. Chuang, *Quantum Computation and Quantum Information*, Cambridge University Press (2000)

[51] M. Howard, J. Twamley, C. Wittmann, T. Gaebel, F. Jelezko and J. Wrachtrup, *Quantum process tomography of a single solid state qubit*, New J. Phys. Vol 8 (2006) 33

[52] T.F. Havel, J. Math. Phys. 44 (2003) 534

[53] Greiner W and Muller B, *Quantum Mechanics: Symmetries*, Berlin: Springer (1989)

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