CLASSIFICATION OF COMPLETELY POSITIVE MAPS

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ABSTRACT. We define a completely positive map and classify all completely positive linear maps. We further classify all such maps that are trace-preserving and consider their natural applications and relevance to quantum mechanics.

1. INTRODUCTION

Quantum mechanics is perhaps the primary triumph of 20th century physics. It is used in every subfield of physics and has broad applications to the other sciences and engineering. It is the way the microscopic world works.

Without going into the full details of the remarkable range of quantum phenomena, to say the least the world of quantum mechanics is very strange and different from the "classical" world in which we live most directly. Famous and confirmed phenomena include particles tunneling through walls, teleportation of states, paths of light that are neither taken nor not taken, apparent correlations faster than the speed of light and so on. But we do not see most of these effects in the classical macroscopic world—somehow as systems interact with their environment at sufficiently large scales, quantum systems become classical. Why this happens remains a mystery to physicists, but how this breakdown occurs can be theoretically explained and observed. Doing so leads naturally to an examination of completely positive maps.

Mathematical preliminaries and a definition of completely positive maps are presented in Section 2, followed by a full motivation and discussion from the perspective of quantum mechanics in Section 3. These completely positive maps can also be completely classified, as we do in Section 4. Finally in Section 5 we give an example of their applications to quantum noise.

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2. BACKGROUND

2.1. **Positive matrices.** Denoting the space of $n \times n$ matrices with complex entries by $\mathbb{M}_n$, we call a matrix $A \in \mathbb{M}_n$ *positive* if it is positive-semidefinite, that is if it satisfies $x^*Ax \geq 0$ for all $x \in \mathbb{C}^n$, or equivalently if it is Hermitian and all its eigenvalues are non-negative, or if there exists some matrix B such that it can be written $A = B^*B$.

The *spectral theorem* says that any positive matrix $A \in \mathbb{M}_n$ may be written in the spectral decomposition

$$A = \sum_{i=1}^{n} \lambda_i v_i v_i^*, \tag{1}$$

where each λ_i is an eigenvalue of A and the vectors $v_i \in \mathbb{C}^n$ form an orthonormal set of eigenvectors of A. We can also absorb each λ_i into v_i.

The map $\Phi : \mathbb{M}_n \to \mathbb{M}_k$ is called *positive* if for all positive $A \in \mathbb{M}_n$, $\Phi(A)$ is also positive.

2.2. **Completely positive maps.** We denote the space of $m \times m$ block matrices $[[A_{ij}]]$ with entries $A_{ij} \in \mathbb{M}_n$ by $\mathbb{M}_m(\mathbb{M}_n)$. Then the map Φ induces another linear map $\Phi_m : \mathbb{M}_m(\mathbb{M}_n) \to \mathbb{M}_m(\mathbb{M}_k)$ defined by

$$\Phi_m([[A_{ij}]]) = [[\Phi(A_{ij})]]. \tag{2}$$

If the map Φ_m is positive, we say Φ is *m-positive*. Thus a positive map is 1-positive. If Φ is m-positive for all $m \in \mathbb{Z}^+$, we say Φ is *completely positive*.

Example 1. *The transpose operation $\Phi : \mathbb{M}_n \to \mathbb{M}_n$ given by $\Phi(A) = A^T$ is positive but not completely positive.*

The characteristic polynomial for A is given by

$$\det[A - \lambda I].$$

Since $\det A = \det A^T$, *the characteristic polynomial for $\Phi(A)$ is*

$$\det[A^T - \lambda I] = \det[A - \lambda I]^T = \det[A - \lambda I].$$

Thus A and $\Phi(A)$ share the same eigenvalues, so if A is positive so is $\Phi(A)$. Thus Φ is positive.

Now consider action of Φ_2 on the positive matrix

$$A = \begin{bmatrix} \frac{1}{2} & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 & \frac{1}{2} \end{bmatrix} \tag{3}$$

which has characteristic polynomial $\lambda^3(\lambda - 1)$.

$$\Phi_2(A) = \begin{bmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} \end{bmatrix} \tag{4}$$

has characteristic polynomial $(\lambda - \frac{1}{2})^3(\lambda + \frac{1}{2})$, and thus the nonnegative eigenvalue $-\frac{1}{2}$, so it is not positive. Accordingly Φ is not 2-positive, and not completely positive either.

2.3. **Tensor products.** Let $\mathbb{C}^{n\times k}$ be the set of $n \times k$ matrices with complex entries. The *tensor product* of matrices $A \in \mathbb{C}^{n\times k}$ and $B \in \mathbb{C}^{m\times l}$, $A \otimes B \in \mathbb{C}^{n\times k} \otimes \mathbb{C}^{m\times l}$, is defined as

$$A \otimes B = \begin{bmatrix} a_{11}B & a_{12}B & \dots \\ a_{21}B & a_{22}B & \\ \vdots & & \ddots \end{bmatrix}, \tag{5}$$

where a_{ij} denotes the ijth entry of A.

The tensor product provides a natural way to combine matrices to form a new matrix sharing some of those properties. For instance, if $A \in \mathbb{M}_n$ and $B \in \mathbb{M}_m$ are positive, so is $A \otimes B$.

Proof. Let A and B be positive. First of all, as both A and B are Hermitian,

$$(A \otimes B)^* = \begin{bmatrix} \overline{a}_{11}B^* & \overline{a}_{21}B^* & \dots \\ \overline{a}_{12}B^* & \overline{a}_{22}B^* & \\ \vdots & & \ddots \end{bmatrix} = \begin{bmatrix} a_{11}B & a_{12}B & \dots \\ a_{21}B & a_{22}B & \\ \vdots & & \ddots \end{bmatrix} = A \otimes B, \tag{6}$$

so $A \otimes B$ is Hermitian as well.

Then by the spectral theorem, there exist orthonormal sets of eigenvectors x_i and y_j for A and B respectively corresponding to eigenvalues λ_i and μ_j, for $1 \leq i \leq n$ and $1 \leq j \leq m$. Considering x_i and y_j as column matrices, it can be easily verified that

$$(A \otimes B)(x_i \otimes y_j) = \lambda_i \mu_j (x_i \otimes y_j), \tag{7}$$

so $x_i \otimes y_j$ are eigenvectors of $A \otimes B$ with eigenvalues $\lambda_i \mu_j$. As these eigenvectors $x_i \otimes y_j$ are orthogonal and span $\mathbb{C}^{mn}$, all eigenvectors of $A \otimes B$ may be written as $\lambda_i \mu_j$ for some i and j. Then since $\lambda_i \geq 0$ and $\mu_j \geq 0$ implies $\lambda_i \mu_j \geq 0$, the eigenvalues of $A \otimes B$ are non-negative, so $A \otimes B$ is positive. $\square$

We can also define the tensor product of maps. The tensor product $\Theta \otimes \Phi : \mathbb{M}_m \otimes \mathbb{M}_n \to \mathbb{M}_p \otimes \mathbb{M}_k$ of $\Theta : \mathbb{M}_m \to \mathbb{M}_p$ and $\Phi : \mathbb{M}_n \to \mathbb{M}_k$ is given by

$$(\Theta \otimes \Phi)(B \otimes A) = \Theta(B) \otimes \Phi(A). \tag{8}$$

Consider the map $I_m \otimes \Phi : \mathbb{M}_m \otimes \mathbb{M}_n \to \mathbb{M}_p \otimes \mathbb{M}_k$ given by

$$(I_m \otimes \Phi)(B \otimes A) = B \otimes \Phi(A), \tag{9}$$

where I_m is the identity on $\mathbb{M}_m$. Then on $\mathbb{M}_n \otimes \mathbb{M}_n$, the set of matrices $D \in \mathbb{M}_m(\mathbb{M}_n)$ that can be factored as $D = B \otimes A$, we have $I_m \otimes \Phi = \Phi_m$.

This definition is still uniquely defined when extended to all D if we insist on linearity. Let the standard basis for $\mathbb{C}^n$ is given by e_j, so the set $E_{ij} = e_i e_j^*$ is a basis for $\mathbb{M}_n$. Then

$$(I_m \otimes \Phi)(E_{ij} \otimes A_{ij}) = E_{ij} \otimes \Phi(A_{ij}), \tag{10}$$

so we have $(I_m \otimes \Phi)([[A_{ij}]]) = [[\Phi(A_{ij})]]$ for any D with only one non-zero A_{ij}. By linearity, it holds for any sum of such matrices, so it holds for any $[[A_{ij}]] \in \mathbb{M}_n$ simultaneously, which is exactly the definition of Φ_m. Thus equivalently to Eq. 2 we may write

$$\Phi_m = I_m \otimes \Phi. \tag{11}$$

3. Quantum mechanics

A positive matrix is called a *density matrix* if it has trace 1. Density matrices form the set of all quantum states. In the real world, many quantum systems exist in infinite dimensional spaces, but in practice little is lost by treating the number of dimensions n as finite. Closed quantum systems with density matrices $A \in \mathbb{M}_n$ evolve by transitions Φ specified by a unitary matrix U,

$$\Phi(A) = UAU^*. \tag{12}$$

In the case of density matrices, the constraints that the matrices are positive and trace 1 ensure that the eigenvalues form a probability distribution, as the trace is equal to the sum of the eigenvalues for positive matrices. Since conjugation by a unitary matrix preserves eigenvalues, this probability distribution remains the same in closed quantum systems.

In general, we would like to consider a broader range of transitions, the full manner in which one density matrix may be mapped onto another. This includes cases in which the probability distribution is changed, or even when the dimensionality of the system changes, corresponding to the addition or removal of particles from the system.

3.1. **Physical motivations.** In this section, we describe the physical constraints that lead to a full classification of these operations.[1] Let $A \in \mathbb{M}_n$ be a density matrix and consider $\Phi : \mathbb{M}_n \to \mathbb{M}_k$.

[1] The hypotheses in this section are as presented by Nielsen and Chuang, Section 8.2 [3].

First of all, $\Phi(A)$ must still be a density matrix. Then clearly Φ is positive and we require $\operatorname{Tr}\Phi(A) = 1$.

Applying the operation to states separately and then mixing them should be equivalent to applying the operation to states mixed first. Physically, we mix a set of density matrices $\{A_i\}$ by associating a probability distribution $\{p_i\}$, where p_i indicates the probability of finding the state A_i in the new ensemble, and creating the new density matrix

$$A' = \sum_i p_i A_i. \tag{13}$$

A' is a density matrix as $x^* A' x = \sum_i p_i x^* A_i x \geq 0$ and $\operatorname{Tr} A' = \sum_i p_i \operatorname{Tr} A_i = 1$ as the trace is linear. Accordingly, we must have

$$\Phi\left(\sum_i p_i A_i\right) = \sum_i p_i \Phi\left(A_i\right). \tag{14}$$

This constraint is known as *convex linearity*.

Finally, the operation should remain the same even if we consider a larger physical system than that described by A. Let $B \in \mathbb{M}_m$ be another density matrix that is an ancillary system to A. Two systems may be physically combined into one system by looking at the tensor product $B \otimes A$. We already showed that $B \otimes A$ is positive, and as

$$\operatorname{Tr}[B \otimes A] = \sum_{i=1}^{m} b_{ii} \operatorname{Tr} A = \operatorname{Tr} A = 1, \tag{15}$$

it has trace 1, so it is a valid density matrix.

Then the operator Φ_m is the only appropriate extension of Φ to the combined system, as it takes $A \to \Phi(A)$ and $B \to B$ when acting on states that can be written $B \otimes A$:

$$\Phi_m(B \otimes A) = (I_m \otimes \Phi)(B \otimes A) = B \otimes \Phi(A). \tag{16}$$

But any positive $D \in \mathbb{M}_m(\mathbb{M}_n)$ with trace 1 is a valid density matrix for the combined system, whether or not it factors as $D = B \otimes A$. Then as Φ_m is the unique linear extension of $I_m \otimes \Phi$ to $\mathbb{M}_m(\mathbb{M}_n)$, the operation $\Phi_m(D)$ must yield a valid density matrix. Since this must remain true when considering an ancillary system of any size, Φ_m must be positive for all $m \in \mathbb{Z}^+$. Thus Φ must be completely positive.

3.2. **Equivalent constraints.** The requirement that $\operatorname{Tr} \Phi(A) = 1$ for all density matrices A may be extended to the constraint that Φ is *trace-preserving*, that $\operatorname{Tr} A = \operatorname{Tr} \Phi(A)$ for all $A \in \mathbb{M}_n$, as on the set of trace 1 matrices the action of Φ is identical.

Likewise, we may extend the constraint of convex linearity among density matrices to linearity when considering all $A \in \mathbb{M}_n$, as any linear combination of density matrices $A' = \sum_i p_i A_i$ is only a density matrix if it is a convex linear combination since $\operatorname{Tr} A' = \sum_i p_i \operatorname{Tr} A_i = \sum_i p_i = 1$.

4. Classification theorems

4.1. **Completely positive linear maps.** The following two theorems, due originally to Man-Duon Choi [2] are commonly known as "Choi's Theorem." Together they classify all completely positive linear maps.

Theorem 1. *For all $V_j \in \mathbb{C}^{n\times k}$, the map $\Phi : \mathbb{M}_n \to \mathbb{M}_k$ given by*

$$\Phi(A) = \sum_{j=1}^{l} V_j^* A V_j \tag{17}$$

is completely positive.

Proof. From Eq. 2 it is clear that the sum of m-positive maps is an m-positive map. Accordingly we will show that the map $\Phi : \mathbb{M}_n \to \mathbb{M}_k$ given by $\Phi(A) = V^* A V$ is completely positive and thus all maps of the form given by Eq. 17 are completely positive.

For $[[A_{ij}]] \in \mathbb{M}_m(\mathbb{M}_n)$,

$$\Phi_m([[A_{ij}]]) = [[V^* A_{ij} V]] = (I_m \otimes V^*)[[A_{ij}]](I_m \otimes V). \tag{18}$$

Let $x \in \mathbb{C}^{nk}$. Then

$$x^* \Phi_m([[A_{ij}]])x = y^*[[A_{ij}]]y, \tag{19}$$

where $y = (I_m \otimes V)x \in \mathbb{C}^{mn}$. Then if $[[A_{ij}]]$ is positive, $y^*[[A_{ij}]]y \geq 0$ for all $y \in \mathbb{C}^{mn}$, so $\Phi_m([[A_{ij}]])$ is positive as well. Since this holds for all $m \in \mathbb{Z}^+$, Φ is completely positive. $\square$

This next theorem is the heart of the classification proof.

Theorem 2. *Let $\Phi : \mathbb{M}_n \to \mathbb{M}_k$ be a completely positive linear map. Then there exist $V_j \in \mathbb{C}^{n \times k}$, $1 \leq j \leq nk$, such that*

$$\Phi(A) = \sum_{j=1}^{nk} V_j^* A V_j \tag{20}$$

for all $A \in \mathbb{M}_n$.

Proof. We follow the proof given by Bhatia [1], following the lines of Choi's original proof.

Let the standard basis for $\mathbb{C}^n$ be given by e_r. Then as before, the set $E_{rs} = e_r e_s^*$ spans $\mathbb{M}_n$. We will show that if Φ is completely positive, for all E_{rs}, $\Phi(E_{rs})$ must be of the form given by Eq. 20, and accordingly so for $\Phi(A)$ for all $A \in \mathbb{M}_n$.

First, consider a vector $v \in \mathbb{C}^{nk}$. We can write it as the column vector

$$v = \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} \qquad \text{with } x_r \in \mathbb{C}^k, \tag{21}$$

and identify it with the $k \times n$ matrix

$$V^* = [x_1, \ldots, x_n]. \tag{22}$$

Then

$$V^* E_{rs} V = [x_1, \ldots, x_n] e_r e_s^* [x_1, \ldots, x_n]^* = x_r x_s^* \tag{23}$$

and thus

$$vv^* = [[x_r x_s^*]] = [[V^* E_{rs} V]], \tag{24}$$

where the notation $[[A_{rs}]]$ denotes as before the matrix with elements given by the sub-matrices A_{rs}.

Now consider the matrix $[[E_{rs}]] \in \mathbb{M}_n(\mathbb{M}_n)$. This matrix is positive, as

$$[[E_{rs}]] = [[e_r e_s^*]] = uu^*, \tag{25}$$

where

$$u = \begin{bmatrix} e_1 \\ \vdots \\ e_n \end{bmatrix}. \tag{26}$$

Then as Φ is completely positive, it must be n-positive, so $\Phi_n([[E_{rs}]])$ must be positive.

By the spectral theorem, we can write $\Phi_n([[E_{rs}]])$ in the spectral decomposition

$$\Phi_n([[E_{rs}]]) = \sum_{j=1}^{nk} v_j v_j^*, \tag{27}$$

for some $v_j \in \mathbb{C}^{nk}$. Then from Eq. 24, we have

$$\Phi_n([[E_{rs}]]) = \sum_{j=1}^{nk} [[V^* E_{rs} V]]. \tag{28}$$

Now following from the definition of Φ_n, we must have

$$\Phi(E_{rs}) = \sum_{j=1}^{nk} V^* E_{rs} V \tag{29}$$

for all unit matrices E_{rs}. Since Φ is linear, this form holds for all $A \in \mathbb{M}_n$. $\square$

Since every matrix of the form of Eq. 20 is also completely positive by the proceeding theorem, we have further shown in the proof of this theorem that if a map is n-positive, it is completely positive.

4.2. **Trace preserving maps.** Density matrices are the set of positive matrices with trace 1. We can further classify all maps between density matrices as the following theorems show.

Theorem 3. *Let $\Phi : \mathbb{M}_n \to \mathbb{M}_k$ be a map as described in Theorem 1 with the additional constraint for the $\{V_j\}$ that*

$$\sum_{j=1}^{l} V_j V_j^* = I_n, \tag{30}$$

where I_n is the identity matrix on M_n. Then Φ is trace-preserving.

Proof. Since the trace is linear and invariant under cyclic permutations (that is $\operatorname{Tr} AB = \operatorname{Tr} BA$),

$$\operatorname{Tr} \Phi(A) = \operatorname{Tr} \left[\sum_{j=1}^{l} V_j^* A V_j \right] \tag{31}$$

$$= \sum_{j=1}^{l} \operatorname{Tr}[V_j^* A V_j] \tag{32}$$

$$= \sum_{j=1}^{l} \operatorname{Tr}[V_j V_j^* A] \tag{33}$$

$$= \operatorname{Tr} \left[\sum_{j=1}^{l} V_j V_j^* A \right] \tag{34}$$

$$= \operatorname{Tr} A, \tag{35}$$

as desired. □

It is clear that unitary conjugation of the form of Eq. 12 satisfies Theorem 3, so appropriately it remains a valid quantum state transition. But clearly a much broader class of transformations satisfies these results as well. For instance, any probabilistic combination of unitary operations U_j with probabilities p_j (specified by the elements $\sqrt{p_j} U_j$) also satisfies Eq. 30.

Theorem 4. *Let $\Phi : \mathbb{M}_n \to \mathbb{M}_k$ be a completely positive linear map that is also trace preserving. Then the $\{V_j\}$ as used in Theorem 1 also must satisfy*

$$I_n = \sum_{j=1}^{l} V_j V_j^*. \tag{36}$$

Proof. Writing $\Phi(A)$ in the form given by Eq. 17,

$$\operatorname{Tr} A = \operatorname{Tr}\left[\sum_{j=1}^{l} V_j V_j^* A\right], \tag{37}$$

by following the same algebra used from Eq. 31-34. Now let

$$B = \sum_{j=1}^{l} V_j V_j^*, \tag{38}$$

so we have

$$\operatorname{Tr} A = \operatorname{Tr}[BA]. \tag{39}$$

This form holds for all $A \in \mathbb{M}_n$, so consider $A = E_{rs}$ where $E_{rs} = e_r e_s^*$ is the matrix unit element as before. $\operatorname{Tr} E_{rs} = 1$ only if $r = s$, so B has the value 1 along the diagonal. As $r \neq s$ implies $\operatorname{Tr} E_{rs} = 0$, each of the off-diagonal elements of B must be zero. Thus $B = I_n$. □

4.3. **Unitary freedom.** Just as the spectral decomposition of a matrix does not uniquely specify vectors v_i, the operators V_j as described by Theorem 2 (and further by Theorem 4) are not unique. We present this final ancillary result without proof.

Theorem 5. *The set $\{W_j\}$, $W_j \in \mathbb{C}^{n\times k}$ describe the same map Φ as given by $\{V_j\}$ if and only if*

$$W_i = \sum_{j=1}^{l} u_{ij} V_j \tag{40}$$

for some unitary $U \in \mathbb{M}_{nk}$ with entries u_{ij}.

5. Quantum noise

The exact nature of quantum to classical transitions has come to renewed prominence within the past decade or so in the context of interest in quantum information theory and quantum computing. In particular, in principle quantum computers offer tremendously increased speed to solve certain computational problems by the use of closed quantum systems. But in the laboratory no systems are truly closed, and some procedure of quantum error correction must be devised to preserve the power of these algorithm. To do so requires a rigorous understanding of quantum noise, as described by completely positive maps.

The most common form of quantum noise is *phase damping*. It is characterized by the off-diagonal elements of a density matrix going to 0. Since this process is irreversible, there is no representation for this operation by unitary conjugation in the form of Eq. 12. Two-level quantum systems known as *qubits* are the building blocks of quantum computers, so this is the base case for of any family of quantum operations. Then process of phase damping on an element of $\mathbb{M}_2$ in the form of Eq. 17 is given by matrices V_j

$$\begin{bmatrix} 1 & 0 \\ 0 & \sqrt{1-\gamma} \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} 0 & 0 \\ 0 & \sqrt{\gamma} \end{bmatrix}, \tag{41}$$

for some γ such that $0 \leq \gamma \leq 1$. It is easy to verify that this map satisfies the constraints of Eq. 36 and performs the transformation

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix} \rightarrow \begin{bmatrix} a & b\lambda \\ c\lambda & d \end{bmatrix}. \tag{42}$$

where $\lambda = \sqrt{1-\gamma}$ is some damping factor. Accordingly we can describe any degree of phase damping on a single qubit. We can extend this process to any quantum system in $\mathbb{M}_{2^n}$ by either writing new operation elements, or taking the tensor product of this map with itself n times. The procedure for other types of quantum noise is similar.

6. Further reading

A detailed discussion of completely positive maps and further results are given by Bhatia in "Positive Definite Matrices" [1]. For proof of these results in the mathematical language of physicists, and extensive discussion of their applications to quantum mechanics, a good reference is Neilsen and Chuang's "Quantum Computation and Quantum Information" [3], especially Chapter 8.

References

[1] Rajendra Bhatia. *Positive Definite Matrices*. Princeton Series in Applied Mathematics. Princeton University Press, Princeton and Oxford, 2007.

[2] Man-Duen Choi. Completely positive linear maps on complex matrices. *Linear Algebra and its Applications*, 10:285–290, 1975.

[3] Michael A. Nielsen and Isaac L. Chaung. *Quantum Computation and Quantum Information*. Cambridge University Press, Cambridge, UK, 2000.