

Higher-order quantum transformations: From quantum circuit design to indefinite causal order

Lecture I. The higher-order quantum formalism: Channels and superchannels

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1 Introduction

Higher-order quantum transformations are operations whose inputs and outputs are not necessarily quantum states, but rather possibly *supermaps* that themselves act on quantum states, such as quantum channels [1–5]. Also called *supermaps*, one typical example is the higher-order transformation that takes a quantum channel as input and outputs another quantum channel, often referred to as a *superchannel*.

These operations are usually defined by linearity and (complete) admissibility, i.e, (multi-)linear mappings from the set of inputs to the set of outputs. The requirement of admissibility can be phrased in terms of universality of the transformation: any element of the input set must be mapped to an element in the output set. In quantum terms this means that a superchannel must transform any arbitrary quantum channel, which can be unknown and hence treated as a black-box, into a valid quantum channel, regardless of its classical description. The requirement of complete admissibility can be phrased as imposing that the higher-order transformation maps all valid inputs to valid outputs, even when acting on only “part” of the input. For example, a superchannel maps all bipartite quantum channels into bipartite (here also called “extended”) quantum channels, even when acting on only one part of the channel.

Further examples of transformations that can be viewed as higher-order quantum operations are:

- States $\rightarrow$ Probability distributions (Quantum measurements)
- Channels $\rightarrow$ Channels (Superchannels)
- Channels $\rightarrow$ Probabilities (Testers)
- Superchannels $\rightarrow$ Superchannels (Adapters)
- ...

2 Basic elements

In quantum theory:

- **Data** (0th-order object): Quantum States

$$\rho \in \mathcal{L}(\mathcal{H})$$

- **Functions** (1st-order object): Quantum Channels

$$\tilde{C} : \mathcal{L}(\mathcal{H}_I) \rightarrow \mathcal{L}(\mathcal{H}_O)$$

$$\tilde{C}(\rho) = \rho'$$

- **Functions of functions** (2nd-order object): Quantum Superchannels

$$\tilde{\tilde{S}} : [\mathcal{L}(\mathcal{H}_I) \rightarrow \mathcal{L}(\mathcal{H}_O)] \rightarrow [\mathcal{L}(\mathcal{H}_{I'}) \rightarrow \mathcal{L}(\mathcal{H}_{O'})]$$

$$\tilde{\tilde{S}}(\tilde{C}) = \tilde{C}'$$

3 Quantum channels

3.1 Quantum states

A quantum state is represented by a linear operator $\rho \in \mathcal{L}(\mathcal{H})$ that satisfies

$$\rho \geq 0 \quad \text{and} \quad \text{tr}(\rho) = 1. \quad (1)$$

3.2 Quantum channels

Quantum channels are linear maps $\tilde{C}(\rho) : \mathcal{L}(\mathcal{H}_I) \rightarrow \mathcal{L}(\mathcal{H}_O)$, where $\mathcal{H}_I$ denotes the Hilbert space of an input system and $\mathcal{H}_O$ of an output system, that preserve the properties of quantum states:

- $\forall \rho \in \mathcal{L}(\mathcal{H}_I)$ such that $\text{tr}(\rho) = 1$, we have that $\text{tr}(\tilde{C}(\rho)) = 1$: Trace-preserving **(TP)** map.
- $\forall \rho \in \mathcal{L}(\mathcal{H}_I)$ such that $\rho \geq 0$, we have that $\tilde{C}(\rho) \geq 0$: Positive **(P)** map.

Is this enough? No. Consider the transposition map $\tilde{C}(\rho) = \rho^T$. It is trace-preserving and positive. However, if acting on part of a two-qubit entangled state $\rho = |\phi^+\rangle\langle\phi^+| \in \mathcal{L}(\mathcal{H}_A \otimes \mathcal{H}_B)$, where $|\phi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$, the resulting state

$$\tilde{C} \otimes \mathbb{1}(\rho) = \rho^{T_A} \quad (2)$$

has eigenvalues $\{-1/2, 1/2, 1/2, 1/2\}$, hence it is not positive semidefinite.

Thus, we require quantum channels to satisfy

- $\forall \rho \in \mathcal{L}(\mathcal{H}_I \otimes \mathcal{H})$ such that $\text{tr}(\rho) = 1$, we have that $\text{tr}[\tilde{C} \otimes \mathbb{1}(\rho)] = 1$: Completely trace-preserving **(CTP)** map.
- $\forall \rho \in \mathcal{L}(\mathcal{H}_I \otimes \mathcal{H})$ such that $\rho \geq 0$, we have that $\tilde{C} \otimes \mathbb{1}(\rho) \geq 0$: Completely positive **(CP)** map.

Note that:

$$\tilde{C} \text{ is CTP} \iff \tilde{C} \text{ is TP}$$

$$\tilde{C} \text{ is CP} \implies \tilde{C} \text{ is P} \quad \text{but} \quad \tilde{C} \text{ is P} \not\Leftarrow \tilde{C} \text{ is CP}$$

Therefore, quantum channels are represented by completely positive trace-preserving (**CPTP**) maps.

3.3 Characterization of CPTP maps

1. **Kraus representation:** For every quantum channel $\tilde{C} : \mathcal{L}(\mathcal{H}_I) \rightarrow \mathcal{L}(\mathcal{H}_O)$, there exists a set of operators $\{K_i\}$, with $K_i : \mathcal{H}_I \rightarrow \mathcal{H}_O$ satisfying $\sum_i K_i^\dagger K_i = \mathbb{1}$, such that:

$$\tilde{C}(\rho) = \sum_i K_i \rho K_i^\dagger \quad (3)$$

This decomposition is not unique.

— A channel is called **isometric** if it can be represented by a set of Kraus operators that contains a single element $V : \mathcal{H}_I \rightarrow \mathcal{H}_O$, with $V^\dagger V = \mathbb{1}$, such that

$$\tilde{V}(\rho) = V \rho V^\dagger. \quad (4)$$

If $\mathcal{H}_I \cong \mathcal{H}_O \cong \mathcal{H}$, then an isometric channel is referred to as a **unitary** channel $\tilde{U}(\rho) = U \rho U^\dagger$, where $U : \mathcal{H} \rightarrow \mathcal{H}$ is a unitary operator satisfying $U^\dagger U = U U^\dagger = \mathbb{1}$.

2. **Stinespring representation:** Following the Stinespring dilation theorem, every quantum channel $\tilde{C} : \mathcal{L}(\mathcal{H}_I) \rightarrow \mathcal{L}(\mathcal{H}_O)$ can be represented by an isometric quantum channel $\tilde{V} : \mathcal{L}(\mathcal{H}_I) \rightarrow \mathcal{L}(\mathcal{H}_O \otimes \mathcal{H}_E)$, where $\mathcal{L}(\mathcal{H}_E)$ represents an environment system, followed by a partial trace on $\mathcal{H}_E$, according to

$$\tilde{C}(\rho) = \text{tr}_E \left(\tilde{V}(\rho) \right) = \text{tr}_E (V \rho V^\dagger), \quad (5)$$

where $V : \mathcal{H}_I \rightarrow \mathcal{H}_O \otimes \mathcal{H}_E$ can be constructed from the Kraus operators $\{K_i\}$ of $\tilde{C}$ according to

$$V = \sum_i K_i \otimes |i\rangle \quad (6)$$

where $\{|i\rangle\}_i$ is the computational basis of $\mathcal{H}_E$. The Stinespring dilation of a quantum channel, often referred to as the purification of the quantum channel, is not unique (but unique up to an isometry acting on the environment).

3. **Choi representation:** Using the Choi-Jamiołkowski isomorphism, any linear map $\tilde{C} : \mathcal{L}(\mathcal{H}_I) \rightarrow \mathcal{L}(\mathcal{H}_O)$ can be represented by a linear operator $C \in \mathcal{L}(\mathcal{H}_I \otimes \mathcal{H}_O)$ that acts on the joint input and output spaces, called the *Choi operator*, which is defined as

$$C := \sum_{ij} |i\rangle\langle j| \otimes \tilde{C}[|i\rangle\langle j|], \quad (7)$$

where $\{|i\rangle\}_i$ is the computational basis on $\mathcal{H}_I$. A linear map $\tilde{C}$ is CP if and only

$$C \geq 0, \quad (8)$$

and is TP if and only if C satisfies

$$\text{tr}_O(C) = \mathbb{1}_I, \quad (9)$$

where $\mathbb{1}_I$ is the identity operator acting on $\mathcal{L}(\mathcal{H}_I)$. Hence, the Choi operator of quantum channels is completely characterized by these two conditions. Then, the output of a quantum channel

$\rho' = \tilde{C}(\rho)$ can be written in terms of the Choi operator C of the map $\tilde{C}$ according to

$$\rho' = \tilde{C}(\rho) = \text{tr}_I[C(\rho^T \otimes \mathbb{1}_O)], \quad (10)$$

where $(\cdot)^T$ denotes transposition with respect to the computational basis. Given a choice of computational basis and a linear map, its Choi operator is a *unique* description of the linear map.

— **Isometric** quantum channels $\tilde{V} : \mathcal{L}(\mathcal{H}_I) \rightarrow \mathcal{L}(\mathcal{H}_O)$ have a rank-one Choi operator represented as $|V\rangle\langle V| \in \mathcal{L}(\mathcal{H}_I \otimes \mathcal{H}_O)$, defined by

$$|V\rangle := \sum_i |i\rangle \otimes V|i\rangle. \quad (11)$$

Notice that the Choi operator of a pure channel $|V\rangle\langle V|$ has $\text{tr}(|V\rangle\langle V|) = d_I$, where $d_I := \dim(\mathcal{H}_I)$.

3.4 The link product and the trace-and-replace map

The composition of maps in the Choi representation is given by the **link product** [1]. Using this representation, the composition $\tilde{G} \circ \tilde{F}$ of two maps $\tilde{F} : \mathcal{L}(\mathcal{H}_1) \rightarrow \mathcal{L}(\mathcal{H}_2)$ and $\tilde{G} : \mathcal{L}(\mathcal{H}_2) \rightarrow \mathcal{L}(\mathcal{H}_3)$, with respective Choi operators $F \in \mathcal{L}(\mathcal{H}_1 \otimes \mathcal{H}_2)$ and $G \in \mathcal{L}(\mathcal{H}_2 \otimes \mathcal{H}_3)$, is given by the *link product* $F * G \in \mathcal{L}(\mathcal{H}_1 \otimes \mathcal{H}_3)$, according to

$$\tilde{G} \circ \tilde{F} = F * G := \text{tr}_2[(F^{T_2} \otimes \mathbb{1}_3)(\mathbb{1}_1 \otimes G)], \quad (12)$$

where $(\cdot)^{T_X}$ denotes partial transposition with respect to the computational basis of $\mathcal{H}_X$.

Note that both the partial transposition and the partial trace are taken over the overlapping linear spaces of F and G . More generally, the link product can be used to compose any two operators A and B :

- If $A \in \mathcal{L}(\mathcal{H}_1)$ and $B \in \mathcal{L}(\mathcal{H}_2)$, then $A * B = A \otimes B \in \mathcal{L}(\mathcal{H}_1 \otimes \mathcal{H}_2)$.
- If $A, B \in \mathcal{L}(\mathcal{H}_1)$, then $A * B = \text{tr}(A^T B) \in \mathbb{C}$.

Consequently, we can see that the output state of a quantum channel $\rho' = \tilde{C}(\rho)$ can be represented with the link product as well, according to

$$\rho' = \tilde{C}(\rho) = C * \rho. \quad (13)$$

The link product satisfies the following properties [1]:

- Commutative: $A * B = B * A$ (does not imply the commutativity of the underlying linear maps).
- Associative: $A * (B * C) = (A * B) * C$.
- Preserves positive semidefiniteness: $A * B \geq 0$ for all $A \geq 0$ and $B \geq 0$.

Let us also define the **trace-and-replace map**, which will be a useful short-hand notation later. Given any operator $A \in \mathcal{L}(\mathcal{H}_X \otimes \mathcal{H})$, we define

$${}_X A := \text{tr}_X(A) \otimes \frac{\mathbb{1}_X}{d_X}, \quad (14)$$

where $d_X := \dim(\mathcal{H}_X)$. Notice that the trace-and-replace map is self-adjoint, that is,

$$\text{tr}_X({}_X A B) = \text{tr}_X(A {}_X B). \quad (15)$$

Given this, we can express the conditions for an operator to be the Choi operator of a quantum channel, i.e. $C \geq 0$ and $\text{tr}_O(C) = \mathbb{1}_I$, in the following form,

$$C \geq 0 \quad (16)$$

$$\text{tr}(C) = d_I \quad (17)$$

$$C = \mathbb{P}_{\text{Chan}}(C) := C - {}_OC + {}_IO C, \quad (18)$$

where $\mathbb{P}_{\text{Chan}}$ is the projector onto the subspace of Choi operators of TP maps. Therefore, the set of all valid quantum channels in their Choi form can be defined as

$$\text{Channel} := \{C \in \mathcal{L}(\mathcal{H}_I \otimes \mathcal{H}_O) \mid C \geq 0, \text{tr}(C) = d_I, C = \mathbb{P}_{\text{Chan}}(C)\}. \quad (19)$$

4 Quantum Superchannels

Superchannels are the most general linear supermaps that transform every input quantum channel into another quantum channel, even when acting on part of the input channel.

More formally,

Definition 1 (Single-slot superchannel). *A superchannel is a linear supermap $\tilde{S} : [\mathcal{L}(\mathcal{H}_I) \rightarrow \mathcal{L}(\mathcal{H}_O)] \rightarrow [\mathcal{L}(\mathcal{H}_P) \rightarrow \mathcal{L}(\mathcal{H}_F)]$, such that, for every quantum channel $\tilde{C}_{\text{ext}} : \mathcal{L}(\mathcal{H}_I \otimes \mathcal{H}_{I'}) \rightarrow \mathcal{L}(\mathcal{H}_O \otimes \mathcal{H}_{O'})$, where $\mathcal{L}(\mathcal{H}_{I'})$ and $\mathcal{L}(\mathcal{H}_{O'})$ are auxiliary input and output systems, one has that*

$$\tilde{S} \otimes \tilde{\mathbb{1}}(\tilde{C}_{\text{ext}}) = \tilde{C}'_{\text{ext}}, \quad (20)$$

where $\tilde{C}'_{\text{ext}} : \mathcal{L}(\mathcal{H}_P \otimes \mathcal{H}_{I'}) \rightarrow \mathcal{L}(\mathcal{H}_F \otimes \mathcal{H}_{O'})$ is also a quantum channel, and where $\tilde{\mathbb{1}}$ is the identity supermap acting on $[\mathcal{L}(\mathcal{H}_{I'}) \rightarrow \mathcal{L}(\mathcal{H}_{O'})] \rightarrow [\mathcal{L}(\mathcal{H}_{I'}) \rightarrow \mathcal{L}(\mathcal{H}_{O'})]$.

Hence, superchannels are linear and **completely CPTP preserving maps**.

In the case of input channels that do not act on auxiliary systems, denoting a channel $\tilde{C} : \mathcal{L}(\mathcal{H}_I) \rightarrow \mathcal{L}(\mathcal{H}_O)$ with its Choi operator $C \in \mathcal{L}(\mathcal{H}_I \otimes \mathcal{H}_O)$ allows us to view the supermap $\tilde{S}$ as a map $\tilde{S} : \mathcal{L}(\mathcal{H}_I \otimes \mathcal{H}_O) \rightarrow \mathcal{L}(\mathcal{H}_P \otimes \mathcal{H}_F)$, such that $\tilde{S}(C) = C' \in \mathcal{L}(\mathcal{H}_P \otimes \mathcal{H}_F)$. Finally, since now the superchannel is given by a linear map, we can write it in the Choi representation as an operator $S \in \mathcal{L}(\mathcal{H}_P \otimes \mathcal{H}_I \otimes \mathcal{H}_O \otimes \mathcal{H}_F)$ such that $C' = \tilde{S}(C)$ is given by

$$C' = \tilde{S}(C) = S * C = \text{tr}_{IO}[(C^T \otimes \mathbb{1}_{PF}) S]. \quad (21)$$

The case of general quantum channels that act on auxiliary systems works analogously. Denoting a channel $\tilde{C}_{\text{ext}}$ with its Choi operator $C_{\text{ext}} \in \mathcal{L}(\mathcal{H}_I \otimes \mathcal{H}_{I'} \otimes \mathcal{H}_O \otimes \mathcal{H}_{O'})$ allows us to view the supermap $\tilde{S}$ as a map $\tilde{S} : \mathcal{L}(\mathcal{H}_I \otimes \mathcal{H}_O) \rightarrow \mathcal{L}(\mathcal{H}_P \otimes \mathcal{H}_F)$, such that $\tilde{S} \otimes \tilde{\mathbb{1}}(C_{\text{ext}}) = C'_{\text{ext}} \in \mathcal{L}(\mathcal{H}_P \otimes \mathcal{H}_{I'} \otimes \mathcal{H}_F \otimes \mathcal{H}_{O'})$. Finally, since now the superchannel is given by a linear map, we can write it in the Choi picture as an operator $S \in \mathcal{L}(\mathcal{H}_P \otimes \mathcal{H}_I \otimes \mathcal{H}_O \otimes \mathcal{H}_F)$ such that $C'_{\text{ext}} = \tilde{S} \otimes \tilde{\mathbb{1}}(C_{\text{ext}})$ is given by

$$C'_{\text{ext}} = \tilde{S} \otimes \tilde{\mathbb{1}}(C_{\text{ext}}) = S * C_{\text{ext}} = \text{tr}_{IO}[(C_{\text{ext}}^{T_{IO}} \otimes \mathbb{1}_{PF}) (\mathbb{1}_{I'O'} \otimes S)]. \quad (22)$$

We can now characterize the Choi operator of superchannels in terms of positivity constraints and linear constraints.

Proposition 1 (Characterization of superchannels). *A linear operator $S \in \mathcal{L}(\mathcal{H}_P \otimes \mathcal{H}_I \otimes \mathcal{H}_O \otimes \mathcal{H}_F)$ represents a superchannel, i.e., is an operator such that, for every Choi state of an extended quantum channel $C_{\text{ext}} \in \mathcal{L}(\mathcal{H}_I \otimes \mathcal{H}_{I'} \otimes \mathcal{H}_O \otimes \mathcal{H}_{O'})$, one has that $S * C_{\text{ext}} = C'_{\text{ext}} \in \mathcal{L}(\mathcal{H}_P \otimes \mathcal{H}_{I'} \otimes \mathcal{H}_F \otimes \mathcal{H}_{O'})$ is*

also an extended quantum channel, if and only if

$$S \geq 0 \quad (23)$$

$$\text{tr}(S) = d_P d_O \quad (24)$$

$$\text{tr}_F(S) = \text{tr}_{OF}(S) \otimes \frac{\mathbb{1}_O}{d_O} \quad (25)$$

$$\text{tr}_{IOF}(S) = \text{tr}(S) \frac{\mathbb{1}_P}{d_P}. \quad (26)$$

Notice that Eqs. (24) and (26) can be equivalently expressed together as

$$\text{tr}_{IOF}(S) = d_O \mathbb{1}_P. \quad (27)$$

Proof. In order to guarantee that $\tilde{S}$ is a superchannel, two conditions must be imposed on its Choi: (i) complete CP preservation ($S * C_{\text{ext}} \geq 0, \forall C_{\text{ext}} \geq 0$), here called the positivity condition, and (ii) complete TP preservation ($\text{tr}_{O'F}[S * C_{\text{ext}}] = \mathbb{1}_{P'} \forall C_{\text{ext}}; \text{tr}_{OO'}[C_{\text{ext}}] = \mathbb{1}_{I'}$), here called the normalization condition.

- Positivity:

$$\begin{aligned} C'_{\text{ext}} = \tilde{S} \otimes \tilde{\mathbb{1}}(C_{\text{ext}}) &\geq 0 \quad \forall C_{\text{ext}} \geq 0 \\ &\iff \\ S &\geq 0. \end{aligned} \quad (28)$$

By definition, $\tilde{S}$ must be a completely positive map. The proof of the above implication then follows from Choi's theorem, which states that the Choi operator of a completely positive map is a positive semidefinite operator.

In fact, to obtain the above condition, complete CP preservation is necessary, as imposing only CP preservation ($\tilde{S}(C) \geq 0, \forall C \geq 0$, for quantum channels without auxiliary systems) does not imply that $S \geq 0$: the complete CP preservation condition is not equivalent to the CP preservation condition.

On the other hand, complete TP preservation ($\text{tr}_{O'F}[S * C_{\text{ext}}] = \mathbb{1}_{P'} \forall C_{\text{ext}}; \text{tr}_{OO'}[C_{\text{ext}}] = \mathbb{1}_{I'}$) and TP preservation ($\text{tr}_F[S * C] = \mathbb{1}_P \forall C; \text{tr}_O[C] = \mathbb{1}_I$, for quantum channels without auxiliary systems), are equivalent conditions. We start by analyzing the condition of TP preservation.

- Normalization:

$$\begin{aligned} \text{tr}_F(C') = \text{tr}_F(S * C) &= \text{tr}_{IOF}[(C^T \otimes \mathbb{1}_{PF}) S] = \mathbb{1}_P \quad \forall C; \text{tr}_O(C) = \mathbb{1}_I \\ &\iff \\ \text{tr}_F(S) &= \text{tr}_{OF}(S) \otimes \frac{\mathbb{1}_O}{d_O} \quad \text{and} \quad \text{tr}_{IOF}(S) = d_O \mathbb{1}_P. \end{aligned} \quad (29)$$

To see the $\Leftarrow$ implication, it can be checked via direct calculation that if $\text{tr}_F(S) = \text{tr}_{OF}(S) \otimes \frac{\mathbb{1}_O}{d_O}$

and $\text{tr}_{IOF}(S) = d_O \mathbb{1}_P$, then

$$\text{tr}_{IOF}[(C^T \otimes \mathbb{1}_{PF}) S] = \text{tr}_{IO}[(C^T \otimes \mathbb{1}_P) \text{tr}_F(S)] \quad (30)$$

$$= \text{tr}_{IO}[(C^T \otimes \mathbb{1}_P) (\text{tr}_{OF}(S) \otimes \frac{\mathbb{1}_O}{d_O})] \quad (31)$$

$$= \frac{1}{d_O} \text{tr}_I[(\text{tr}_O(C^T) \otimes \mathbb{1}_P) (\text{tr}_{OF}(S))] \quad (32)$$

$$= \frac{1}{d_O} \text{tr}_I[(\mathbb{1}_I \otimes \mathbb{1}_P) (\text{tr}_{OF}(S))] \quad (33)$$

$$= \frac{1}{d_O} \text{tr}_{IOF}(S) \quad (34)$$

$$= \mathbb{1}_P, \quad (35)$$

where we used the fact that $\text{tr}_O(C^T) = \text{tr}_O(C) = \mathbb{1}_I$.

To see the $\Rightarrow$ implication, we start by taking C to be parametrized by a Hermitian operator X according to $C = X - OX + \frac{\mathbb{1}}{d_O}$ [4]. Since transposition leaves the set of Hermitian operators invariant, we can also write $C^T = X - OX + \frac{\mathbb{1}}{d_O}$ for some $X = X^\dagger$.

Substituting this in, one gets that $\text{tr}_{IOF}[(C^T \otimes \mathbb{1}_{PF}) S] = \mathbb{1}_P$ is equivalent to

$$\text{tr}_{IOF} \left[\left(\left(X - OX + \frac{\mathbb{1}}{d_O} \right) \otimes \mathbb{1}_{PF} \right) S \right] = \mathbb{1}_P \quad \forall X = X^\dagger. \quad (36)$$

We can split this into two cases: $X = 0$ and $X \neq 0$.

For $X = 0$:

$$\text{tr}_{IOF} \left[\left(\left(X - OX + \frac{\mathbb{1}}{d_O} \right) \otimes \mathbb{1}_{PF} \right) S \right] = \text{tr}_{IOF} \left(\frac{S}{d_O} \right) = \mathbb{1}_P \iff \text{tr}_{IOF}(S) = d_O \mathbb{1}_P. \quad (37)$$

For $X \neq 0$:

$$\text{tr}_{IOF} \left[\left(\left(X - OX + \frac{\mathbb{1}}{d_O} \right) \otimes \mathbb{1}_{PF} \right) S \right] = \text{tr}_{IOF} [(X - OX) \otimes \mathbb{1}_{PF}] S + \text{tr}_{IOF} \left(\frac{S}{d_O} \right) = \mathbb{1}_P, \quad (38)$$

from which we get that

$$\text{tr}_{IOF} [(X - OX) \otimes \mathbb{1}_{PF}] S = 0 \quad (39)$$

$$\text{tr}_{IO} [(X \otimes \mathbb{1}_P) \text{tr}_F(S)] - \text{tr}_{IO} [(OX \otimes \mathbb{1}_P) \text{tr}_F(S)] = 0 \quad (40)$$

$$\text{tr}_{IO} [(X \otimes \mathbb{1}_P) \text{tr}_F(S)] - \text{tr}_{IO} [(X \otimes \mathbb{1}_P) O \text{tr}_F(S)] = 0 \quad (41)$$

$$\text{tr}_{IO} [(X \otimes \mathbb{1}_P) (\text{tr}_F(S) - O \text{tr}_F(S))] = 0 \quad (42)$$

$$\iff \text{tr}_F(S) - O \text{tr}_F(S) = 0, \quad \text{or, equivalently,} \quad (43)$$

$$\text{tr}_F(S) - \text{tr}_{OF}(S) \otimes \frac{\mathbb{1}_O}{d_O} = 0. \quad (44)$$

Finally, to check that these conditions are equivalent to complete TP preservation, one can follow the

same steps as above with the starting point being

$$\begin{aligned} \text{tr}_{O'F}(C'_{\text{ext}}) &= \text{tr}_{O'F}(S * C_{\text{ext}}) = \text{tr}_{IOO'F}[(C_{\text{ext}}^{T_I T_O} \otimes \mathbb{1}_{PF}) (\mathbb{1}_{I'O'} \otimes S)] = \mathbb{1}_{PI'} \quad \forall C_{\text{ext}}; \quad \text{tr}_{OO'}(C_{\text{ext}}) = \mathbb{1}_{II'} \\ &\iff \\ \text{tr}_F(S) &= \text{tr}_{OF}(S) \otimes \frac{\mathbb{1}_O}{d_O} \quad \text{and} \quad \text{tr}_{IOF}(S) = d_O \mathbb{1}_P. \end{aligned} \tag{45}$$

□

Notice that, using the trace-and-replace notation, the characterization of a superchannel in Eqs. (23)–(26) can be equivalently rewritten as

$$S \geq 0 \tag{46}$$

$$\text{tr}(S) = d_P d_O \tag{47}$$

$$_F S = _O F S \tag{48}$$

$$_{IOF} S = _{PIOF} S, \tag{49}$$

or even, combining the last two constraints into a projector, one arrives at

$$S \geq 0 \tag{50}$$

$$\text{tr}(S) = d_P d_O \tag{51}$$

$$S = \mathbb{P}_{\text{SChan}}(S) := S - _F S + _O F S - _{IOF} S + _{PIOF} S, \tag{52}$$

where $\mathbb{P}_{\text{SChan}}$ is the projector onto the subspace of Choi operators of (completely) TP preserving maps. The set of valid superchannels is then

$$\text{SChannel} := \{S \in \mathcal{L}(\mathcal{H}_P \otimes \mathcal{H}_I \otimes \mathcal{H}_O \otimes \mathcal{H}_F) \mid S \geq 0, \text{tr}(S) = d_P d_O, S = \mathbb{P}_{\text{SChan}}(S)\}. \tag{53}$$

We now show that every superchannel can be realized by a quantum circuit.

Proposition 2 (Quantum-circuit realization of superchannels). *A linear supermap $\tilde{S} : [\mathcal{L}(\mathcal{H}_I) \rightarrow \mathcal{L}(\mathcal{H}_O)] \rightarrow [\mathcal{L}(\mathcal{H}_P) \rightarrow \mathcal{L}(\mathcal{H}_F)]$ with Choi operator $S \in \mathcal{L}(\mathcal{H}_P \otimes \mathcal{H}_I \otimes \mathcal{H}_O \otimes \mathcal{H}_F)$ corresponds to a superchannel if and only if there exists an “encoder” quantum channel $\tilde{E} : \mathcal{L}(\mathcal{H}_P) \rightarrow \mathcal{L}(\mathcal{H}_I \otimes \mathcal{H}_M)$, with Choi operator $E \in \mathcal{L}(\mathcal{H}_P \otimes \mathcal{H}_I \otimes \mathcal{H}_M)$, where $\mathcal{L}(\mathcal{H}_M)$ represents a memory system, and a “decoder” quantum channel $\tilde{D} : \mathcal{L}(\mathcal{H}_M \otimes \mathcal{H}_O) \rightarrow \mathcal{L}(\mathcal{H}_F)$, with Choi operator $D \in \mathcal{L}(\mathcal{H}_M \otimes \mathcal{H}_O \otimes \mathcal{H}_F)$, such that*

$$\tilde{S} \otimes \mathbb{1}(\tilde{C}) = \tilde{D} \circ (\mathbb{1} \otimes \tilde{C}) \circ \tilde{E}, \tag{54}$$

or, in terms of the Choi operators,

$$S = E * D = \text{tr}_M[(E^{T_M} \otimes \mathbb{1}_{OF})(\mathbb{1}_{PI} \otimes D)]. \tag{55}$$

Proof. To prove this statement, we begin by showing, via direct calculation, that every S in the form of Eq. (55) satisfies Eqs. (23)–(26). Recall that it follows from the properties of the link product that $S = E * D \geq 0$ since $E \geq 0$ and $D \geq 0$. Additionally, recall that since E and D are Choi operators of quantum channels, they satisfy $\text{tr}_{IM}(E) = \mathbb{1}_P$ and $\text{tr}_F(D) = \mathbb{1}_{MO}$.

Then, to show that for every S that satisfy Eqs. (23)–(26), there exist quantum channels E and D such that Eq. (55) holds, we take the following Ansatz: Let $\sigma := \text{tr}_{OF}(S)/d_O$ be embedded in $\mathcal{L}(\mathcal{H}_M)$,

where $\mathcal{H}_M \cong \mathcal{H}_P \otimes \mathcal{H}_I$. Then,

$$E := \left(\mathbb{1}_{PI} \otimes \sqrt{\sigma^T} \right) \sum_{ij} |ii\rangle\langle jj| \left(\mathbb{1}_{PI} \otimes \sqrt{\sigma^T} \right) \quad (56)$$

$$D := \left(\sqrt{\sigma}^{-1} \otimes \mathbb{1}_{OF} \right) S \left(\sqrt{\sigma}^{-1} \otimes \mathbb{1}_{OF} \right), \quad (57)$$

where $\sqrt{A}$ denotes the unique positive square root of $A \geq 0$ and A^{-1} denotes the Moore-Penrose (pseudo)inverse. By direct calculation, it can be verified that (i) E is a valid quantum channel in the Choi representation, (ii) D is also valid quantum channel in the Choi representation, and (iii) $D * E = S$, concluding the proof. $\square$

4.1 Pure superchannels

Pure superchannels are the ones that have a rank-1 Choi operator. While not every superchannel is pure, every superchannel can be purified.

Notice that, by construction, E in Eq. (56) is rank-1 and the Choi operator of an isometric channel, so it can be written as $E = |V_E\rangle\langle V_E|$ with $|V_E\rangle = (\mathbb{1}_{PI} \otimes \sqrt{\sigma^T}) \sum_i |ii\rangle$ taken directly from Eq. (56). On the other hand, D in Eq. (57) is not necessarily rank-1 by construction, and hence, not the Choi operator of an isometric channel. Nevertheless, applying the Stinespring dilation theorem, D can be purified according to

$$|V_D\rangle = (\mathbb{1}_{AOF} \otimes \sqrt{D}) \sum_i |ii\rangle, \quad (58)$$

such that $|V_D\rangle\langle V_D| \in \mathcal{L}(\mathcal{H}_M \otimes \mathcal{H}_O \otimes \mathcal{H}_F \otimes \mathcal{H}_E)$, where $\mathcal{H}_E \cong \mathcal{H}_M \otimes \mathcal{H}_O \otimes \mathcal{H}_F$, satisfies

$$\text{tr}_E |V_D\rangle\langle V_D| = D. \quad (59)$$

Hence, any superchannel S can be expressed as a rank one operator given by $|V_E\rangle\langle V_E| * |V_D\rangle\langle V_D|$ followed by a partial trace, according to

$$S = \text{tr}_E(|V_E\rangle\langle V_E| * |V_D\rangle\langle V_D|). \quad (60)$$

This fact can be interpreted as a sort of Stinespring-like dilation/purification theorem for superchannels. Pure superchannels are the ones in which D in Eq. (57) is already isometric, and consequently one can take $d_E = 1$.

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