Necessary and Sufficient Conditions on Measurements of Quantum Channels

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Quantum supermaps are a higher-order generalization of quantum maps, taking quantum maps to quantum maps. It is known that any completely positive, trace non-increasing (CPTNI) map can be performed as part of a quantum measurement. By providing an explicit counterexample we show that, instead, not every quantum supermap sending a quantum channel to a CPTNI map can be realized in a measurement on quantum channels. We find that the supermaps that can be implemented in this way are exactly those transforming quantum channels into CPTNI maps even when tensored with the identity supermap. We link this result to the fact that the principle of causality fails in the theory of quantum supermaps.

1. INTRODUCTION

One of the most puzzling aspects of quantum mechanics has always been the need to consider probabilistic processes to describe the observation of physical systems. The development of quantum information theory has turned this puzzling feature into a resource for many protocols. Think, for instance, of the implementation of quantum computation through measurements (measurement-based quantum computation) [1, 2], of quantum cryptographic protocols [3–6], or of the generation of random numbers [7].

Focusing our attention on finite-dimensional quantum systems, the most general quantum measuring device can be described by a set of linear maps that are completely positive and trace non-increasing (CPTNI). The maps in this set must sum to a quantum channel, namely to a completely positive and trace-preserving (CPTP) linear map [8–10]. This situation is described by a *quantum instrument* [10–13]: a quantum channel that takes a quantum system as input, and outputs a a classical-quantum system, where the classical system represents the 'meter' read by the experimenter. From the classical outcome read on the meter, one can infer which CPTNI map occurred during the experiment. This characterization of quantum experiments, in conjunction with the fact that quantum channels with trivial (i.e. 1-dimensional) input represent states [14], singles out channels as the fundamental objects of quantum theory, encapsulating all the other processes.

For this reason, it is important to understand how to manipulate quantum channels. The study of such manipulations, initiated in [14–16], has both practical [14, 17–28] and foundational consequences [16, 17, 25, 29–31], and has led to the development of new research areas, such as resource theories of quantum processes [28, 32–55]. The manipulation of quantum channels is implemented by *supermaps* [14–16, 38, 56, 57], which are linear transformations sending linear maps to linear maps. In this setting, *superchannels* [14, 38] represent the way a channel can evolve deterministically, in the same way as channels represent the deterministic evolution of a quantum state. Superchannels are the supermaps that take quantum channels to quantum channels even when tensored with the identity supermap [16]. Measurements on channels are then described by a set of supermaps that sum to a superchannel, giving rise to the notion of a quantum *super-instrument*.

In this article we focus on measurements performed on quantum channels, and we show that a naive application of a condition similar to CPTNI in quantum theory is *not* enough to single out physical supermaps, viz. those that can arise in an experiment performed on quantum channels.

We will adopt the following notation.

Notation. $\mathfrak{B}(\mathcal{H})$ denotes the set of bounded linear operators on the finite-dimensional Hilbert space $\mathcal{H}$, $\mathfrak{B}_h(\mathcal{H})$ the set of bounded hermitian operators on $\mathcal{H}$, and $\mathfrak{D}(\mathcal{H})$ the set of density matrices on $\mathcal{H}$. Every letter without a subscript denotes a pair of systems $A := A_0 A_1$, where A_0 is usually regarded as an input system, and A_1 as an output system. Thus $\mathcal{E}^A := \mathcal{E}^{A_0 \to A_1}$ denotes a linear map with input A_0 and output A_1, and $\mathfrak{L}^A := \mathfrak{L}^{A_0 \to A_1}$ is the set of such linear maps, from $\mathfrak{B}(\mathcal{H}^{A_0})$ to $\mathfrak{B}(\mathcal{H}^{A_1})$. $|A_0|$ denotes the dimension of $\mathcal{H}^{A_0}$. A supermap $\Theta^{A \to B}$ takes elements of $\mathfrak{L}^A$ to elements of $\mathfrak{L}^B$, and its action on a linear map $\mathcal{E}^A$ is denoted with square brackets: $\Theta^{A \to B}\left[\mathcal{E}^A\right]$. Finally, a tilde over
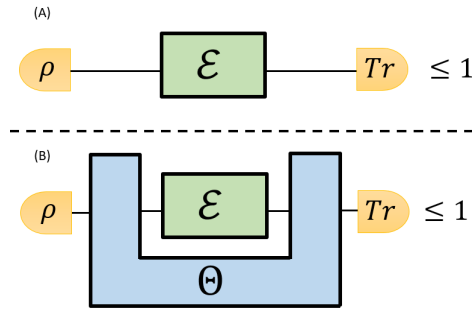

Figure 1. The condition for a CP map $\mathcal{E}$ to be a CPTNI map is represented in (a). The condition for a CPP supermap Θ to be a CPTNI-preserving supermap is depicted in (b). Note that the two conditions are formally very similar, the only difference being the presence of the vice representing the supermap Θ. Therefore, we can rightfully say that CPTNI-preserving supermaps are the higher-level analogy of CPTNI maps.

a system, as in $A_0 \widetilde{A}_0$, indicates that we are considering two identical copies of a system (in this case A_0). We adopt the following convention concerning partial traces: if M^{AB} is a matrix on $A_0 A_1 B_0 B_1$, M^{AB_0} denotes the partial trace on the missing system B_1: $M^{AB_0} := \mathrm{Tr}_{B_1}\left[M^{AB}\right]$. In summary, when a superscript is missing, we have taken the partial trace over the missing system of the original matrix.

2. CPTNI-PRESERVING SUPERMAPS

The first condition one must require of physical supermaps is that they be *completely CP-preserving* (CPP): they should send CP maps to CP maps even when tensored with the identity supermap. In formula, a supermap $\Theta^{A \to B}$ is CPP if for all bipartite CP maps $\mathcal{E}^{RA} \in \mathfrak{L}^{RA}$, we have that

$$\left(\mathbf{1}^R \otimes \Theta^{A \to B}\right)\left[\mathcal{E}^{RA}\right], \tag{2.1}$$

is still a CP map, where $\mathbf{1}^R := \mathbf{1}^{R \to R}$ is the identity supermap. This is analogous to the CP condition for quantum maps.

The second condition, analogous to being TNI for quantum maps, is that a physical supermap should send CPTNI maps to CPTNI maps. If a supermap is CPP, demanding this is equivalent to requiring that it should take *CPTP* maps to CPTNI maps (see appendix A). More precisely, a supermap $\Theta^{A \to B}$ is *CPTNI-preserving* if it is CPP and

$$\mathrm{Tr}\left[\Theta^{A \to B}\left[\mathcal{N}^A\right]\left(\rho^{B_0}\right)\right] \leq 1, \tag{2.2}$$

for any CPTP map $\mathcal{N}^A \in \mathfrak{L}^A$ and any $\rho^{B_0} \in \mathfrak{D}\left(\mathcal{H}^{B_0}\right)$. The analogy between CPTNI quantum maps and CPTNI-preserving supermaps is illustrated in Fig. 1.

A measurement on quantum channels (called a *super-measurement*) is described by a set of CPTNI-preserving supermaps $\left\{\Theta_x^{A \to B}\right\}_{x \in X}$, indexed by the outcome x of the measurement, such that $\sum_{x \in X} \Theta_x^{A \to B}$ is a superchannel. This gives rise to the super-instrument:

$$\Upsilon^{A \to X_1 B}\left[\mathcal{E}^A\right] = \sum_{x \in X} |x\rangle\langle x|^{X_1} \otimes \Theta_x^{A \to B}\left[\mathcal{E}^A\right], \tag{2.3}$$

for every CP map $\mathcal{E}^A$, where system X_1 represents the classical meter and $\left\{|x\rangle^{X_1}\right\}$ is an orthonormal basis of X_1.

Our main result is that, surprisingly, *not all* CPTNI-preserving supermaps can arise in a quantum super-measurement, therefore *not all* CPTNI-preserving supermaps are physical. An example is the supermap $\Theta^{A \to B}$ whose action on a generic CP map $\mathcal{E}^A$ is:

$$\Theta^{A \to B}\left[\mathcal{E}^A\right]\left(\rho^{B_0}\right) = \mathrm{Tr}\left[\mathcal{E}^{A_0 \to B_0}\left(u^{A_0}\right) Y^{B_0}\left(\rho^{B_0}\right)^{\mathrm{T}} Y^{B_0}\right] u^{B_1}, \tag{2.4}$$

where all systems are qubits, u is the maximally mixed state, and Y is the Pauli Y matrix (ρ^{B_0} is a generic density matrix, used to define the action of the CPTNI map $\Theta^{A \to B}\left[\mathcal{E}^A\right]$ on its input). Note that, if $\mathcal{E}^A$ is CPTP, one has indeed $\mathrm{Tr}\left[\Theta^{A \to B}\left[\mathcal{E}^A\right]\left(\rho^{B_0}\right)\right] \leq 1$, because ρ^{B_0} is a density matrix. This means that the supermap $\Theta^{A \to B}$ is CPTNI-preserving (cf. Eq. (2.2)). Full details are presented in appendix C.

3. COMPLETELY CPTNI-PRESERVING SUPERMAPS

We find that the right condition to ensure that a CPTNI-preserving supermap $\Theta^{A \to B}$ is physical is that it be *completely* CPTNI-preserving. This means that it is CPTNI-preserving even when tensored with the identity supermap:

$$\mathrm{Tr}\left[\left(\mathbf{1}^R \otimes \Theta^{A \to B}\right)\left[\mathcal{N}^{RA}\right]\left(\rho^{R_0 B_0}\right)\right] \leq 1, \tag{3.1}$$

where $\mathcal{N}^{RA}$ is a CPTP map, and $\rho^{R_0 B_0} \in \mathfrak{D}\left(\mathcal{H}^{R_0 B_0}\right)$. The example in Eq. (2.4) highlights that, in general, not all CPTNI-preserving supermaps are completely CPTNI-preserving.

For superchannels the situation is different: it is sufficient to demand that they be CPP and TP-preserving (TPP), without requiring that they be TPP in a *complete* sense [38]. The situation of generic supermaps is also different from linear maps acting on quantum states. In the latter case, to have a physical CP map, it is enough to require that it be TNI, without demanding it in a complete sense. The ultimate reason for these different behaviours is related to causality and no-signalling [58], and it is fully examined in appendix F.

4. THE MAIN RESULT

Following [15, 38], we work in the Choi picture for quantum maps and supermaps. A summary of useful facts is presented in appendix B 1. Let $\mathbf{J}_\Theta^{AB}$ be the Choi matrix of a supermap $\Theta^{A \to B}$, and $J_\mathcal{E}^A$ the Choi matrix of a linear map $\mathcal{E}^A \in \mathfrak{L}^A$. Then $\Theta^{A \to B}$ is a CPTNI-preserving supermap if and only if $\mathbf{J}_\Theta^{AB} \geq 0$ (since it is CPP), and it satisfies the additional condition deriving from Eq. (2.2):

$$\mathrm{Tr}\left[\mathbf{J}_\Theta^{AB_0}\left(J_\mathcal{N}^A \otimes \rho^{B_0}\right)^{\mathrm{T}}\right] \leq 1, \tag{4.1}$$

for every CPTP map $\mathcal{N}^A \in \mathfrak{L}^A$, and every $\rho^{B_0} \in \mathfrak{D}\left(\mathcal{H}^{B_0}\right)$ (see appendix B 1). Notice the similarity with the definition of CPTNI maps $\mathcal{E}$ in the Choi picture, namely

$$\mathrm{Tr}\left[J_\mathcal{E}^A\left(\left(\rho^{A_0}\right)^{\mathrm{T}} \otimes I^{A_1}\right)\right] \leq 1,$$

for every $\rho^{A_0} \in \mathfrak{D}\left(\mathcal{H}^{A_0}\right)$.

In a similar spirit, we can express the requirement of complete CPTNI preservation in Eq. (3.1) in the Choi picture as $\mathbf{J}_\Theta^{AB} \geq 0$ plus the remarkably simple additional constraint

$$\mathrm{Tr}\left[\mathbf{J}_\Theta^{AB_0}\left(M^{AB_0}\right)^{\mathrm{T}}\right] \leq 1, \tag{4.2}$$

for every positive semi-definite matrix M^{AB_0} with marginal $M^{A_0 B_0} = I^{A_0} \otimes \rho^{B_0}$, for some $\rho^{B_0} \in \mathfrak{D}\left(\mathcal{H}^{B_0}\right)$. The technical details are provided in appendix B 2.

It is not hard to check that all the matrices of the form $J_\mathcal{N}^A \otimes \rho^{B_0}$, with $\mathcal{N}^A$ CPTP, are a strict subset of the matrices M^{AB_0}, confirming that complete CPTNI preservation is at least as strict a condition as CPTNI preservation. In fact, it is stricter, as our counterexample in Eq. (2.4) shows: the supermap in Eq. (2.4) is CPTNI-preserving but *not completely* CPTNI-preserving. Consequently, the set of completely CPTNI-preserving supermaps is strictly contained in the set of CPTNI-preserving supermaps. The situation is illustrated in Fig. 2.

To obtain our main result, namely the characterization of which CPTNI-preserving supermaps are physical, we consider a semi-definite program (SDP) inspired by Eq. (4.2):

$$\begin{aligned}
\text{Find} \quad & \alpha = \max_M \mathrm{Tr}\left[\mathbf{J}_\Theta^{AB_0}\left(M^{AB_0}\right)^{\mathrm{T}}\right] \\
\text{Subject to:} \quad & M^{AB_0} \geq 0 \\
& M^{A_0 B_0} = I^{A_0} \otimes \rho^{B_0}.
\end{aligned} \tag{4.3}$$

If we consider the dual of the SDP (4.3)

$$\begin{aligned}
\text{Find} \quad & \beta = |A_0| \min r \\
\text{Subject to:} \quad & r|A_0| \mathbf{J}_\Phi^{A_0 B_0} \otimes u^{A_1} \geq \mathbf{J}_\Theta^{AB_0} \\
& \mathbf{J}_\Phi^{A_0 B_0} \geq 0 \\
& \mathbf{J}_\Phi^{A_1 B_0} = I^{A_1 B_0} \\
& r \geq 0 \\
& r \in \mathbb{R} \\
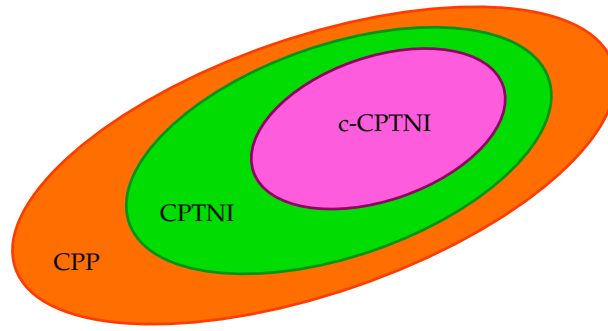& \Phi \text{ superchannel,}
\end{aligned}$$

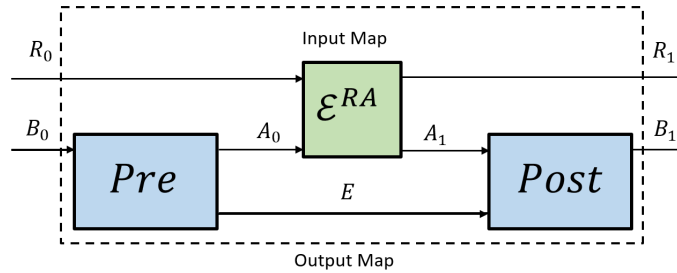Figure 2. Inclusions between sets of supermaps. Here c-CPTNI denotes completely CPTNI-preserving supermaps.

Figure 3. Representation of a completely CPTNI-preserving supermap. Here, a bipartite input map $\mathcal{E}^{RA}$ is inserted between a CPTP pre-processing map and a CPTNI post-processing map. The output is a bipartite CPTNI map. Note the presence of the ancillary system E, which acts as a "memory" between the pre-processing and the post-processing. This realization of a supermap is called a quantum 1-comb [19].

we convert Eq. (4.3) from an SDP having a constraint on M^{AB_0} into one having an explicit condition on $\mathbf{J}_\Theta^{AB_0}$. This condition is exactly what we need to derive our main result.

Theorem 4.1. *A CPTNI-preserving supermap can be completed to a superchannel if and only if it is* completely *CPTNI-preserving.*

The full proof is presented in appendix D.

5.   REALIZATION OF COMPLETELY CPTNI-PRESERVING SUPERMAPS

Using the Choi picture, we can re-obtain a result of [14, theorem 2], namely that every completely CPTNI-preserving supermap can be expressed in terms of a CPTP pre-processing map and a CPTNI post-processing map, as depicted in Fig. 3. In formula, if $\Theta_x^{A\to B}$ is a completely CPTNI-preserving supermap, associated with the outcome x of a quantum super-instrument, its Choi matrix $\mathbf{J}_{\Theta_x}^{AB}$ can be expressed in the following form:

$$\mathbf{J}_{\Theta_x}^{AB} = \left(\mathcal{I}^{AB_0} \otimes \Gamma_{\text{post}_x}^{\widetilde{A}_1 E_0 \to B_1}\right) \circ \left(\mathcal{I}^{A_1 \widetilde{A}_1 B_0} \otimes \Gamma_{\text{pre}}^{\widetilde{B}_0 \to A_0 E_0}\right)\left(\phi_+^{B_0 \widetilde{B}_0} \otimes \phi_+^{A_1 \widetilde{A}_1}\right),$$ (5.1)

where $\mathcal{I}^{AB_0}$ is the identity channel on AB_0 and $\phi_+^{B_0\widetilde{B}_0} = \sum_{j,k}|jj\rangle\langle kk|^{B_0\widetilde{B}_0}$ is the unnormalized maximally entangled state of $B_0\widetilde{B}_0$. Here $\Gamma_{\text{pre}}^{\widetilde{B}_0 \to A_0 E_0}$ is the CPTP pre-processing map, and $\Gamma_{\text{post}_x}^{\widetilde{A}_1 E_0 \to B_1}$ is the CPTNI post-processing map. Being that $\Theta_x^{A\to B}$ is part of a quantum super-instrument, we also have that $\sum_x \Gamma_{\text{post}_x}^{\widetilde{A}_1 E_0 \to B_1}$ is a CPTP map. The proof of this result is reported in appendix E. Note that the pre-processing $\Gamma_{\text{pre}}^{\widetilde{B}_0 \to A_0 E_0}$ is independent of x, therefore it can be chosen to be the same for all the supermaps in the same super-instrument.

6. THE ROLE OF CAUSALITY

To summarize, for the first time we exactly pinned down the necessary and sufficient conditions determining which supermaps can appear in quantum super-instruments. Specifically, we found that only completely CPTNI-preserving supermaps can be implemented in a quantum super-instrument. Additionally, we showed an explicit example of a supermap that is CPTNI-preserving, but not completely CPTNI-preserving (Eq. (2.4)). Viewing CPTNI preservation as a higher-order generalization of the CPTNI condition for quantum maps (cf. Fig. 1), we cannot fail to note the difference between the theory of quantum supermaps—where CPTNI maps are regarded as states—and quantum theory. Indeed, in quantum theory, all CPTNI maps $\mathcal{E}^A$ are also *completely* CPTNI, the latter meaning:

$$\text{Tr}\left[\left(\mathcal{I}^{R_0} \otimes \mathcal{E}^A\right)\left(\rho^{R_0 A_0}\right)\right] \leq 1, \tag{6.1}$$

for every $\rho^{R_0 A_0} \in \mathfrak{D}\left(\mathcal{H}^{R_0 A_0}\right)$. The ultimate reason for this difference is that the theory of quantum supermaps does not satisfy the fundamental property of causality [58].

Axiom 6.1 (Causality). *The probability of a transformation occurring in an experiment is independent of the choice of experiments performed on its output.*

Loosely speaking, causality means that information cannot "come back from the future". One of its consequences is that all bipartite states are non-signalling. The existence of signalling bipartite channels [59, 60] is a clear signature that causality does not hold in the theory of quantum supermaps. Moreover, we can get an intuitive grasp of the failure of causality from the realization of physical supermaps expressed in Eq. (5.1) and in Fig. 3. Consider a super-measurement $\left\{\Theta_x^{A \to B}\right\}$ performed on a CPTNI map $\mathcal{E}^A$, which means that the measurement occurs *after* $\mathcal{E}^A$ is prepared in a laboratory or in a quantum circuit. The presence of pre-processing in the realization of every $\Theta_x^{A \to B}$ implies that $\Theta_x^{A \to B}$ acts on the *input* of $\mathcal{E}^A$ too, meaning, in some sense, that part of $\Theta_x^{A \to B}$ also acts *before* $\mathcal{E}^A$. Somehow in this situation there is *not* a well-defined notion of what comes "before" and "after", so causality cannot hold; for it would select a clear "arrow of time" in information processing.

More precisely, causality can be proved to be equivalent to the existence of a unique way to discard a physical system deterministically [58, 61–63], corresponding to the deterministic POVM $\{I\}$ in quantum theory, viz. taking the (partial) trace. However, if we want to discard a quantum channel deterministically, we need to resort to deterministic process POVMs [64], which are highly non-unique. More specifically, all deterministic process POVMs can be realized as the quantum circuit fragments

$$\boxed{\rho}\!-\!\!\overset{A_0}{\quad}\qquad \overset{A_1}{\quad}\!\!-\!\boxed{\text{Tr}}\,,$$

for any choice of quantum state $\rho^{A_0} \in \mathfrak{D}\left(\mathcal{H}^{A_0}\right)$, where the channel is put in the slot (see appendix F 1). This tells us that the theory of quantum supermaps is non-causal. In particular, for bipartite channels there are some *entangled* deterministic process POVMs:

$$\left.\rho\right\rangle\!\!\begin{array}{c} \overset{A_0}{\quad}\qquad \overset{A_1}{\quad}\!\!-\!\boxed{\text{Tr}}\\ \overset{B_0}{\quad}\qquad \overset{B_1}{\quad}\!\!-\!\boxed{\text{Tr}}\end{array}\,,$$

for $\rho^{A_0 B_0} \in \mathfrak{D}\left(\mathcal{H}^{A_0 B_0}\right)$ entangled. We can collectively call the deterministic ways to discard a physical object (whether a quantum state or a quantum channel) as 'deterministic effects', which will be denoted as u in circuit diagrams. It can be shown that *no* entangled deterministic effects exist in causal theories, where they are in a tensor product form [58]. For example, in quantum theory the deterministic POVM on the composite system $\mathcal{H}^{A_0} \otimes \mathcal{H}^{B_0}$ is $I^{A_0 B_0} = I^{A_0} \otimes I^{B_0}$.

Using operational probabilistic theories [58, 65–67], based on the notion of circuits and on the composition of physical transformations occurring in experiments (see appendix F 1), we can achieve a unified approach to establishing which operations are physical. These will be the operations on the objects of interest (i.e. states or channels) that can arise in a measurement or in a generic experiment done on them. In particular, we obtain the following necessary and sufficient condition valid in any unrestricted theory (e.g. when there are no superselection rules), whether causal or not.

Theorem 6.2. $\mathcal{A}$ *is a physical operation if and only if it is 'completely positive' and*

$$\left.\rho\right\rangle\!\!\begin{array}{c}\overset{A}{\quad}\boxed{\mathcal{A}}\overset{B}{\quad}\\ \overset{S}{\quad}\end{array}\!\!\boxed{u} \leq 1, \tag{6.2}$$

for every system S*, every 'deterministic state'* ρ*, and every deterministic effect* u*.*

Here, by 'deterministic state' we mean the deterministic object we are interested in; it can be a quantum state or a quantum channel. $\mathcal{A}$ represents an operation that is performed on the objects of interest: a quantum map in quantum theory, or a quantum supermap if our objects of interest are quantum channels. 'Completely positive' in this setting means that the operation preserves the convex cone generated by 'states' in a complete sense. For quantum theory, it means that $\mathcal{A}$ is CP; for quantum supermaps that $\mathcal{A}$ is a CPP supermap. Now, let us explain the meaning of Eq. (6.2). In quantum theory, u is nothing but the deterministic POVM, i.e. tracing out both systems, which has a tensor product form due to causality. We obtain the simple TNI condition $\text{Tr}\left[\mathcal{A}\left(\rho\right)\right] \leq 1$ for all quantum states ρ, and not Eq. (6.1). If our objects of interest are, instead, quantum channels, this time u is a deterministic bipartite process POVM. Now, the existence of entangled bipartite process POVMs, a consequence of the *failure of causality*, does *not* allow us to reduce the condition of Eq. (6.2) to a simple condition involving only one system. Therefore, the conditions of 'complete positivity' and Eq. (6.2) imply that $\mathcal{A}$ must be CPP and *completely* CPTNI preserving (Eq. (3.1)), and we cannot get rid of the 'complete sense' required in this condition.

A rigorous proof and statement of this result, along with more details on the implications of causality for the theory of quantum supermaps, is presented in appendix F 2.

7. CONCLUSION

The results we obtained in this article improve our understanding of the operational viewpoint in quantum theory, and more generally in physics. In particular, we showed that the correct conditions to impose on a linear transformation to guarantee its physicality, be it a quantum map or a quantum supermap, must always be formulated in a *complete sense*. This means that they must always involve the tensor product with the identity transformation. Thus, for quantum supermaps we have the CPP condition and the complete CPTNI preservation condition. For quantum maps we have the CP condition and the complete TNI condition of Eq. (6.1). Since quantum theory satisfies causality, Eq. (6.1) becomes *equivalent* to the TNI condition we impose ordinarily on quantum maps. However, the fundamental requirement is still the one expressed by Eq. (6.1). In other words, the existence of signalling bipartite states in the theory of quantum supermaps is the reason for the gap between CPTNI preservation and complete CPTNI preservation; in the very same way as the existence of entangled states in quantum theory creates a gap between positive and completely positive maps, which are instead the same notion in classical physics.

The fact that conditions expressed in a complete sense are the right thing to demand is apparent if one adopts the circuit framework in which operational probabilistic theories are formulated. Our results confirm and strengthen the validity of this approach to the study of the fundamental operational properties of physical theories.

Contributions JB, MG, and CMS did most of the technical work, and contributed equally to the article. CMS wrote most of the article, and had the idea of linking the main result with the principle of causality. GC and GG had the main idea of the article, and provided guidance and direction to the research.

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Appendix A: General facts about quantum maps and supermaps

Quantum maps describe the evolution of quantum systems, in both the deterministic and the probabilistic case (e.g. when a measurement is performed). To be consistent with the interpretation of mixed states as probabilistic ensembles, a quantum map $\mathcal{E}^A$ must be linear, $\mathcal{E}^A \in \mathfrak{L}^A$. This is not enough, because a quantum map must send quantum states to quantum states even when applied only to half of a bipartite state. For this reason we first demand that it be *completely positive* (CP): for every $\rho^{R_0 A_0} \in \mathfrak{D}\left(\mathcal{H}^{R_0 A_0}\right)$ it must be

$$\left(\mathcal{I}^{R_0} \otimes \mathcal{E}^A\right)\left(\rho^{R_0 A_0}\right) \geq 0,$$

where $\mathcal{I}^{R_0}$ is the identity map on system R_0. This means that $\mathcal{E}^A$ sends positive semi-definite operators to positive semi-definite operators even when tensored with the identity. We also require that a map $\mathcal{E}^A$ be *trace non-increasing*

(TNI):

$$\mathrm{Tr}\left[\mathcal{E}^A\left(\rho^{A_0}\right)\right] \leq 1,$$

for every $\rho^{A_0} \in \mathfrak{D}\left(\mathcal{H}^{A_0}\right)$. In particular, if the trace is preserved, that is $\mathrm{Tr}\left[\mathcal{E}^A\left(\rho^{A_0}\right)\right] = 1$, for every $\rho^{A_0} \in \mathfrak{D}\left(\mathcal{H}^{A_0}\right)$, we say that the map is *trace-preserving* (TP). The allowed quantum maps are those that are both CP and TNI (CPTNI). CPTP maps are also called *quantum channels*, and represent the most general deterministic evolutions a quantum system can undergo. CPTNI maps that are not CPTP represent non-deterministic transformations. This is what happens in a quantum measurement, which can be seen as a collection of CPTNI maps $\left\{\mathcal{E}_x^A\right\}$, indexed by the outcomes x of that measurement, such that $\sum_x \mathcal{E}_x^A$ is a CPTP map. If we know the outcome x of the measurement, then we know that the system evolved under the CPTNI map $\mathcal{E}_x^A$. We can therefore construct a *quantum instrument*

$$\mathcal{E}^{A_0 \to X_1 A_1} = \sum_x |x\rangle \langle x|^{X_1} \otimes \mathcal{E}_x^A, \tag{A.1}$$

where $\left\{|x\rangle^{X_1}\right\}$ is an orthonormal basis of system X_1. $\mathcal{E}^{A_0 \to X_1 A_1}$ is a quantum channel with classical-quantum output. Here X_1 is the classical system, recording the measurement outcome. As such, it represents the meter read by the experimenter performing the quantum measurement $\left\{\mathcal{E}_x^A\right\}$.

These notions can be easily generalized to quantum supermaps [14, 15, 56], namely to transformations sending quantum maps to quantum maps. Again, these are linear maps, and an easy translation of the requirements of CP and TNI leads to the requirement of CPP (Eq. (2.1) in the main article) [14, 38] and TNI preservation. Specifically, a map is CPTNI-preserving if it is CPP, and sends CPTNI maps to CPTNI maps:

$$\mathrm{Tr}\left[\Theta^{A \to B}\left[\mathcal{E}^A\right]\left(\rho^{B_0}\right)\right] \leq 1, \tag{A.2}$$

for any CPTNI map $\mathcal{E}^A$ and any $\rho^{B_0} \in \mathfrak{D}\left(\mathcal{H}^{B_0}\right)$. In fact, if $\Theta^{A \to B}$ is CPP, it is enough to require that inequality (A.2) be satisfied by quantum channels $\mathcal{E}^A$, namely by CPTP maps.

To see it, let $\mathcal{E}^A$ be a CPTNI map. We can always find another CPTNI map $\mathcal{E}'^A$ such that $\mathcal{E}^A + \mathcal{E}'^A$ is CPTP. Now assume that $\Theta^{A \to B}$ is CPP, and sends CPTP maps to CPTNI maps. Then, for every $\rho^{B_0} \in \mathcal{D}\left(\mathcal{H}^{B_0}\right)$,

$$1 \geq \mathrm{Tr}\left[\Theta^{A \to B}\left[\mathcal{E}^A + \mathcal{E}'^A\right]\left(\rho^{B_0}\right)\right] = \mathrm{Tr}\left[\Theta^{A \to B}\left[\mathcal{E}^A\right]\left(\rho^{B_0}\right)\right] + \mathrm{Tr}\left[\Theta^{A \to B}\left[\mathcal{E}'^A\right]\left(\rho^{B_0}\right)\right].$$

Since $\Theta^{A \to B}$ is CPP, then $\mathrm{Tr}\left[\Theta^{A \to B}\left[\mathcal{E}^A\right]\left(\rho^{B_0}\right)\right] \geq 0$ and $\mathrm{Tr}\left[\Theta^{A \to B}\left[\mathcal{E}'^A\right]\left(\rho^{B_0}\right)\right] \geq 0$, therefore we conclude that it must be

$$\mathrm{Tr}\left[\Theta^{A \to B}\left[\mathcal{E}^A\right]\left(\rho^{B_0}\right)\right] \leq 1,$$

which means that $\Theta^{A \to B}$ satisfies Eq. (A.2).

A CPTNI-preserving supermap $\Theta^{A \to B}$ is called *superchannel* if it sends CPTP maps to CPTP maps [38]. The original definition in [16] required that it should send quantum channels to quantum channels in a complete sense, i.e. even when tensored with the identity supermap. In other words,

$$\mathrm{Tr}\left[\left(\mathbf{1}^R \otimes \Theta^{A \to B}\right)\left[\mathcal{N}^{RA}\right]\left(\rho^{R_0 B_0}\right)\right] = 1,$$

for any CPTP map $\mathcal{N}^{RA}$ and any $\rho^{R_0 B_0} \in \mathfrak{D}\left(\mathcal{H}^{R_0 B_0}\right)$, where $\mathbf{1}^R$ is the identity supermap on R. Actually, in [38, theorem 1], using the Choi picture, it was proved that we need not consider this requirement in a complete sense: a CPTNI-preserving supermap $\Theta^{A \to B}$ is a superchannel if and only if

$$\mathrm{Tr}\left[\Theta^{A \to B}\left[\mathcal{N}^A\right]\left(\rho^{B_0}\right)\right] = 1, \tag{A.3}$$

for any CPTP map $\mathcal{N}^A$ and any $\rho^{B_0} \in \mathfrak{D}\left(\mathcal{H}^{B_0}\right)$. In Appendix F 2 we will prove this result in an alternative way, without using the Choi isomorphism.

Superchannels are intimately related to channels: it was proved that all superchannels can be represented in terms of a pre- and a post-processing CPTP map [14, 38], as depicted in Fig. 4. Such a representation is called a quantum 1-comb [14].

Superchannels play an important role because they represent all physical ways a quantum channel can evolve in an open system, and provide a framework for measurements on quantum operations, called *super-measurements*. These are described by a set $\left\{\Theta_x^{A \to B}\right\}$ of CPTNI-preserving supermaps such that $\sum_x \Theta_x^{A \to B}$ is a superchannel. Then we
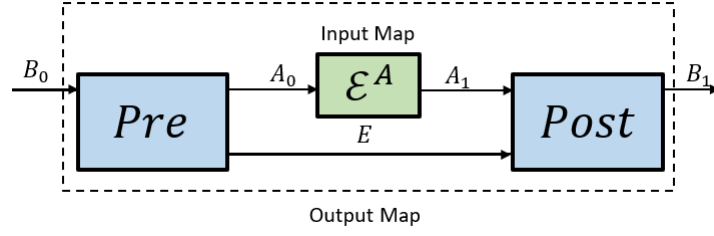
Figure 4. Realization of a superchannel. Here an input quantum channel is inserted between a CPTP pre-processing map and a CPTP post-processing map. The output is another quantum channel. The ancillary system E plays the role of a quantum memory between the pre- and the post-processing.

can construct a *quantum super-instrument* as the generalization of the quantum notion (see Eq. (2.3) in the main article):

$$\Upsilon^{A \to X_1 B} \left[\mathcal{E}^A \right] = \sum_x |x\rangle \langle x|^{X_1} \otimes \Theta_x^{A \to B} \left[\mathcal{E}^A \right],$$

where system X_1 again represents the classical meter, as in Eq. (A.1), and $\mathcal{E}^A$ is any CP map. The main result of this article is that, unlike CPTNI quantum maps, *not all* CPTNI-preserving supermaps can be part of a quantum super-instrument. In Appendix F we link this fact to the failure of causality [58] in the theory of quantum supermaps.

Appendix B: The Choi picture for quantum maps and supermaps

In this appendix we collect some results about the Choi representation of quantum maps and supermaps. Specifically, Appendix B 1 provides the general background information and some basic results about the Choi isomorphism. Appendix B 2 instead focuses on the derivations related to complete CPTNI preservation in the Choi form, and in particular on obtaining Eq. (4.2) in the main article.

1. Choi matrices of quantum maps and supermaps

The first ingredient to define the Choi isomorphism is to consider the super-normalized maximally entangled state $|\phi_+\rangle^{A_0 \widetilde{A}_0} = \sum_{j=1}^{|A_0|} |j\rangle^{A_0} |j\rangle^{\widetilde{A}_0}$, where $\left\{ |j\rangle^{A_0} \right\}$ is a *fixed* orthonormal basis of $\mathcal{H}^{A_0}$ (and therefore of $\mathcal{H}^{\widetilde{A}_0}$ too, since $\widetilde{A}_0$ is just another copy of A_0). The Choi matrix of a linear map $\mathcal{E}^A \in \mathfrak{L}^A$ is defined as

$$J_{\mathcal{E}}^A := \left(\mathcal{I}^{A_0} \otimes \mathcal{E}^{\widetilde{A}_0 \to A_1} \right) \left(\phi_+^{A_0 \widetilde{A}_0} \right),$$

where $\phi_+^{A_0 \widetilde{A}_0} := |\phi_+\rangle \langle \phi_+|^{A_0 \widetilde{A}_0}$, and $\mathcal{I}^{A_0}$ is the identity channel. Again, since $\widetilde{A}_0$ is just another copy of A_0, the linear map $\mathcal{E}^{\widetilde{A}_0 \to A_1}$ is well defined.

In particular, $\mathcal{E}^A$ is CP if and only if $J_{\mathcal{E}}^A \geq 0$. $\mathcal{E}^A$ is CPTP if and only if in addition one has $J_{\mathcal{E}}^{A_0} = I^{A_0}$. Instead, $\mathcal{E}^A$ is CPTNI if and only if, besides $J_{\mathcal{E}}^A \geq 0$, one has $J_{\mathcal{E}}^{A_0} \leq I^{A_0}$. The Choi matrix $J_{\mathcal{E}}^A$ encodes all the information about $\mathcal{E}^A$ because one can reconstruct the action of $\mathcal{E}^A$ on quantum states from its Choi matrix:

$$\mathcal{E}^A \left(\rho^{A_0} \right) = \mathrm{Tr}_{A_0} \left[J_{\mathcal{E}}^A \left(\left(\rho^{A_0} \right)^{\mathrm{T}} \otimes I^{A_1} \right) \right], \tag{B.1}$$

for every $\rho^{A_0} \in \mathfrak{D} \left(\mathcal{H}^{A_0} \right)$.

To define the Choi matrix of a supermap $\Theta^{A \to B}$, we follow the approach presented in [38]. Let us consider the following basis of the space $\mathfrak{L}^A$:

$$\mathcal{E}_{jklm}^A \left(\rho^{A_0} \right) = \langle j|\rho|k\rangle^{A_0} |l\rangle \langle m|^{A_1},$$

for $j, k \in \{1, \ldots, |A_0|\}$ and $l, m \in \{1, \ldots, |A_1|\}$. The Choi matrix of the supermap $\Theta^{A \to B}$ can be defined as

$$\mathbf{J}_\Theta^{AB} := \sum_{j,k,l,m} J_{\mathcal{E}_{jklm}}^A \otimes J_{\Theta[\mathcal{E}_{jklm}]}^B.$$

Again, $\mathbf{J}_\Theta^{AB}$ encodes all the information about $\Theta^{A\to B}$. For instance, $\Theta^{A\to B}$ is CPP if and only if $\mathbf{J}_\Theta^{AB} \geq 0$. Moreover, we can express the action of a supermap on a quantum map $\mathcal{E}^A$ using their Choi matrices: if $\mathcal{F}^B = \Theta^{A\to B}\left[\mathcal{E}^A\right]$, we have [38]:

$$J_{\mathcal{F}}^B = \mathrm{Tr}_A\left[\mathbf{J}_\Theta^{AB}\left(\left(J_{\mathcal{E}}^A\right)^{\mathrm{T}}\otimes I^B\right)\right]. \tag{B.2}$$

A full characterization of superchannels from their Choi matrices was given in [38]: $\Theta^{A\to B}$ is a superchannel if and only if $\mathbf{J}_\Theta^{AB} \geq 0$, and one has $\mathbf{J}_\Theta^{AB_0} = \mathbf{J}_\Theta^{A_0 B_0}\otimes u^{A_1}$ and $\mathbf{J}_\Theta^{A_1 B_0} = I^{A_1 B_0}$. Here $u^{A_1} = \frac{1}{|A_1|}I^{A_1}$ is the maximally mixed state. Combining Eqs. (B.1) and (B.2) for a CPTP map $\mathcal{N}^A$, we have

$$\Theta^{A\to B}\left[\mathcal{N}^A\right]\left(\rho^{B_0}\right) = \mathrm{Tr}_{AB_0}\left[\mathbf{J}_\Theta^{AB}\left(\left(J_{\mathcal{N}}^A\otimes\rho^{B_0}\right)^{\mathrm{T}}\otimes I^{B_1}\right)\right];$$

therefore,

$$\mathrm{Tr}\left[\Theta^{A\to B}\left[\mathcal{N}^A\right]\left(\rho^{B_0}\right)\right] = \mathrm{Tr}_{AB_0}\left\{\mathrm{Tr}_{B_1}\left[\mathbf{J}_\Theta^{AB}\left(\left(J_{\mathcal{N}}^A\otimes\rho^{B_0}\right)^{\mathrm{T}}\otimes I^{B_1}\right)\right]\right\} = \mathrm{Tr}\left[\mathbf{J}_\Theta^{AB_0}\left(J_{\mathcal{N}}^A\otimes\rho^{B_0}\right)^{\mathrm{T}}\right]. \tag{B.3}$$

Hence, by Eq. (A.3) $\Theta^{A\to B}$ is a superchannel if and only if

$$\mathrm{Tr}\left[\mathbf{J}_\Theta^{AB_0}\left(J_{\mathcal{N}}^A\otimes\rho^{B_0}\right)^{\mathrm{T}}\right] = 1.$$

Similarly, we can characterize CPTNI-preserving supermaps in the Choi picture. By Eq. (2.2) in the main article, a supermap is CPTNI-preserving if $\mathrm{Tr}\left[\Theta^{A\to B}\left[\mathcal{N}^A\right]\left(\rho^{B_0}\right)\right] \leq 1$, for every CPTP map $\mathcal{N}^A$ and every density matrix ρ^{B_0}. By Eq. (B.3), we can rewrite this condition in the Choi picture as

$$\mathrm{Tr}\left[\mathbf{J}_\Theta^{AB_0}\left(J_{\mathcal{N}}^A\otimes\rho^{B_0}\right)^{\mathrm{T}}\right] \leq 1.$$

This proves Eq. (4.1) in the main article.

2. Some technical derivations about completely CPTNI-preserving supermaps

Now we will focus on expressing the complete CPTNI preservation condition in the Choi picture. Looking at Eq. (3.1) in the main article tells us that we need to find an expression for $\mathrm{Tr}\left[\left(\mathbf{1}^R\otimes\Theta^{A\to B}\right)\left[\mathcal{N}^{RA}\right]\left(\rho^{R_0 B_0}\right)\right]$ in the Choi picture. Note that the identity supermap does not change the systems it acts on. Therefore, to express Eq. (3.1) in the main article in the Choi form, we only consider how $\mathcal{N}^{RA}$ is acted on by the supermap $\Theta^{A\to B}$, representing the action of the identity superchannel with the identity matrix I^R. Therefore, combining Eqs. (B.1) and (B.2) this time yields:

$$\begin{aligned}\mathrm{Tr}\left[\left(\mathbf{1}^R\otimes\Theta^{A\to B}\right)\left[\mathcal{N}^{RA}\right]\left(\rho^{R_0 B_0}\right)\right] &= \mathrm{Tr}\left[\left(I^R\otimes\mathbf{J}_\Theta^{AB}\right)\left(\left(J_{\mathcal{N}}^{RA}\right)^{\mathrm{T}_A}\otimes I^B\right)\left(\left(\rho^{R_0 B_0}\right)^{\mathrm{T}}\otimes I^{R_1 AB_1}\right)\right] \\ &= \mathrm{Tr}_{R_0 AB_0}\left\{\mathrm{Tr}_{R_1 B_1}\left[\left(I^R\otimes\mathbf{J}_\Theta^{AB}\right)\left(\left(J_{\mathcal{N}}^{RA}\right)^{\mathrm{T}_A}\otimes I^B\right)\left(\left(\rho^{R_0 B_0}\right)^{\mathrm{T}}\otimes I^{R_1 AB_1}\right)\right]\right\} \\ &= \mathrm{Tr}_{R_0 AB_0}\left[\left(I^{R_0}\otimes\mathbf{J}_\Theta^{AB_0}\right)\left(\left(J_{\mathcal{N}}^{R_0 A}\right)^{\mathrm{T}_A}\otimes I^{B_0}\right)\left(\left(\rho^{R_0 B_0}\right)^{\mathrm{T}}\otimes I^A\right)\right]. \tag{B.4}\end{aligned}$$

Now let us define

$$M^{AB_0} := \mathrm{Tr}_{R_0}\left[\left(\rho^{R_0 B_0}\otimes I^A\right)\left(\left(J_{\mathcal{N}}^{R_0 A}\right)^{\mathrm{T}_{R_0}}\otimes I^{B_0}\right)\right], \tag{B.5}$$

and let us calculate:

$$\begin{aligned}\mathrm{Tr}\left[\mathbf{J}_\Theta^{AB_0}\left(M^{AB_0}\right)^{\mathrm{T}}\right] &= \mathrm{Tr}_{R_0 AB_0}\left[\left(I^{R_0}\otimes\mathbf{J}_\Theta^{AB_0}\right)\left(\left(J_{\mathcal{N}}^{R_0 A}\right)^{\mathrm{T}_{R_0}}\otimes I^{B_0}\right)^{\mathrm{T}}\left(\rho^{R_0 B_0}\otimes I^A\right)^{\mathrm{T}}\right] \\ &= \mathrm{Tr}\left[\left(I^{R_0}\otimes\mathbf{J}_\Theta^{AB_0}\right)\left(\left(J_{\mathcal{N}}^{R_0 A}\right)^{\mathrm{T}_A}\otimes I^{B_0}\right)\left(\left(\rho^{R_0 B_0}\right)^{\mathrm{T}}\otimes I^A\right)\right].\end{aligned}$$

As we can see, this coincides with Eq. (B.4). Therefore $\mathrm{Tr}\left[\left(\mathbf{1}^R \otimes \Theta^{A\to B}\right)\left[\mathcal{N}^{RA}\right]\left(\rho^{R_0 B_0}\right)\right] = \mathrm{Tr}\left[\mathbf{J}_\Theta^{AB_0}\left(M^{AB_0}\right)^{\mathrm{T}}\right]$, where M^{AB_0} is defined in Eq. (B.5). Now the complete CPTNI preservation condition of Eq. (3.1) in the main article becomes:

$$\mathrm{Tr}\left[\mathbf{J}_\Theta^{AB_0}\left(M^{AB_0}\right)^{\mathrm{T}}\right] \leq 1, \tag{B.6}$$

for every M^{AB_0} of the form (B.5). Note that $\mathrm{Tr}\left[\mathbf{J}_\Theta^{AB_0}\left(M^{AB_0}\right)^{\mathrm{T}}\right] \geq 0$ for every CPP supermap $\Theta^{A\to B}$, whence M^{AB_0} is positive semi-definite. Furthermore,

$$M^{A_0 B_0} = \mathrm{Tr}_{R_0 A_1}\left[\left(\rho^{R_0 B_0} \otimes I^A\right)\left(\left(J_\mathcal{N}^{R_0 A}\right)^{\mathrm{T}_{R_0}} \otimes I^{B_0}\right)\right] = \mathrm{Tr}_{R_0}\left[\rho^{R_0 B_0}\right] \otimes I^{A_0} = I^{A_0} \otimes \rho^{B_0},$$

where we have used the fact that $\mathrm{Tr}_{R_0 A_1}\left[\left(J_\mathcal{N}^{R_0 A}\right)^{\mathrm{T}_{R_0}}\right] = \mathrm{Tr}_{R_0 A_1}\left[J_\mathcal{N}^{R_0 A}\right]$, and that $\mathrm{Tr}_{A_1}\left[J_\mathcal{N}^{R_0 A}\right] = \mathrm{Tr}_{R_1 A_1}\left[J_\mathcal{N}^{RA}\right] = I^{R_0} \otimes I^{A_0}$ because $\mathcal{N}$ is CPTP (cf. Appendix B 1). So M^{AB_0} has marginal $M^{A_0 B_0} = I^{A_0} \otimes \rho^{B_0}$.

Now we prove a key result, namely that *every* positive semi-definite matrix M^{AB_0} with marginal $M^{A_0 B_0} = I^{A_0} \otimes \rho^{B_0}$, where ρ^{B_0} is any density matrix, can be written as in Eq. (B.5). In this way, instead of stating complete CPTNI preservation as in Eq. (B.6) for M^{AB_0} of the form (B.5), we will state it in a remarkably simpler way: $\Theta^{A\to B}$ is completely CPTNI-preserving if and only if Eq. (B.6) is satisfied for *any* positive semi-definite M^{AB_0} with marginal $M^{A_0 B_0} = I^{A_0} \otimes \rho^{B_0}$. This technical result will be crucial for the main finding of this article, namely the characterization of physical supermaps (see Appendix D).

Lemma B.1. *Let $M^{AB_0} \geq 0$ such that $M^{A_0 B_0} = I^{A_0} \otimes \rho^{B_0}$, for some $\rho^{B_0} \in \mathfrak{D}\left(\mathcal{H}^{B_0}\right)$. Then*

$$M^{AB_0} = \mathrm{Tr}_{R_0}\left[\left(\rho^{R_0 B_0} \otimes I^A\right)\left(\left(J_\mathcal{N}^{R_0 A}\right)^{\mathrm{T}_{R_0}} \otimes I^{B_0}\right)\right],$$

where $\mathcal{N}^{RA}$ is some CPTP map and $\rho^{R_0 B_0} \in \mathfrak{D}\left(\mathcal{H}^{R_0 B_0}\right)$.

Proof. Let $\phi_+^{A_0 \widetilde{A}_0} \otimes \varphi^{E_0 B_0}$ be a purification of $M^{A_0 B_0} = I^{A_0} \otimes \rho^{B_0}$, where $\varphi^{E_0 B_0} \in \mathfrak{D}\left(\mathcal{H}^{E_0 B_0}\right)$ is a purification of ρ^{B_0}. Now let $\tau^{AB_0 F_0}$ be a purification of M^{AB_0}, so $\tau^{AB_0 F_0}$ is also a purification of $M^{A_0 B_0}$. Thus, these two purifications can be related by an isometry channel $\mathcal{V}^{\widetilde{A}_0 E_0 \to A_1 F_0}$ such that [68]

$$\tau^{AB_0 F_0} = \left(\mathcal{I}^{A_0 B_0} \otimes \mathcal{V}^{\widetilde{A}_0 E_0 \to A_1 F_0}\right)\left(\phi_+^{A_0 \widetilde{A}_0} \otimes \varphi^{E_0 B_0}\right).$$

Performing the partial trace on system F_0 yields

$$M^{AB_0} = \left(\mathcal{I}^{A_0 B_0} \otimes \Gamma^{\widetilde{A}_0 E_0 \to A_1}\right)\left(\phi_+^{A_0 \widetilde{A}_0} \otimes \varphi^{E_0 B_0}\right), \tag{B.7}$$

where $\Gamma^{\widetilde{A}_0 E_0 \to A_1} := \mathrm{Tr}_{F_0} \circ \mathcal{V}^{\widetilde{A}_0 E_0 \to A_1 F_0}$ is a CPTP map. The action of $\Gamma^{\widetilde{A}_0 E_0 \to A_1}$ on a generic state $\chi^{\widetilde{A}_0 E_0} \in \mathfrak{D}\left(\mathcal{H}^{\widetilde{A}_0 E_0}\right)$ can be written in terms of its Choi matrix as

$$\Gamma^{\widetilde{A}_0 E_0 \to A_1}\left(\chi^{\widetilde{A}_0 E_0}\right) = \mathrm{Tr}_{\widetilde{A}_0 E_0}\left[J_\Gamma^{\widetilde{A}_0 E_0 A_1}\left(\left(\chi^{\widetilde{A}_0 E_0}\right)^{\mathrm{T}} \otimes I^{A_1}\right)\right]. \tag{B.8}$$

Let us substitute Eq. (B.8) into Eq. (B.7). Note that the identity channel does not change the systems it acts on. Therefore, to express Eq. (B.7) in the Choi form, we only consider how $\phi_+^{A_0 \widetilde{A}_0} \otimes \varphi^{E_0 B_0}$ is acted on by the map $\Gamma^{\widetilde{A}_0 E_0 \to A_1}$, representing the action of the identity channel with the identity matrix $I^{A_0 B_0}$. Thus Eq. (B.7) becomes

$$M^{AB_0} = \mathrm{Tr}_{\widetilde{A}_0 E_0}\left[\left(I^{A_0 B_0} \otimes J_\Gamma^{\widetilde{A}_0 E_0 A_1}\right)\left(\left(\phi_+^{A_0 \widetilde{A}_0}\right)^{\mathrm{T}_{\widetilde{A}_0}} \otimes \left(\varphi^{E_0 B_0}\right)^{\mathrm{T}_{E_0}} \otimes I^{A_1}\right)\right].$$

Expanding $\phi_+^{A_0 \widetilde{A}_0}$, and using the cyclic property of the trace, we get:

$$\mathrm{Tr}_{\widetilde{A}_0 E_0}\left[\left(I^{A_0 B_0} \otimes J_\Gamma^{\widetilde{A}_0 E_0 A_1}\right)\left(\left(\phi_+^{A_0 \widetilde{A}_0}\right)^{\mathrm{T}_{\widetilde{A}_0}} \otimes \left(\varphi^{E_0 B_0}\right)^{\mathrm{T}_{E_0}} \otimes I^{A_1}\right)\right] =$$

$$= \sum_{x,y} |x\rangle \langle y|^{A_0} \otimes \mathrm{Tr}_{E_0} \left[\left(I^{B_0} \otimes \left\langle x \middle| J_\Gamma^{\widetilde{A}_0 E_0 A_1} \middle| y \right\rangle^{\widetilde{A}_0} \right) \left(\left(\varphi^{E_0 B_0} \right)^{\mathrm{T}_{E_0}} \otimes I^A \right) \right].$$

Since $\widetilde{A}_0$ is a copy of A_0,

$$\sum_{x,y} |x\rangle \langle y|^{A_0} \left\langle x \middle| J_\Gamma^{\widetilde{A}_0 E_0 A_1} \middle| y \right\rangle^{\widetilde{A}_0} =: J_\Gamma^{E_0 A},$$

where we have replaced system $\widetilde{A}_0$ with system A_0, and we have set $A := A_0 A_1$ as usual. Now Γ is regarded as a channel from $A_0 E_0$ to A_1. With this in mind, we can write:

$$M^{AB_0} = \mathrm{Tr}_{E_0} \left[\left(J_\Gamma^{E_0 A} \otimes I^{B_0} \right) \left(\left(\varphi^{E_0 B_0} \right)^{\mathrm{T}_{E_0}} \otimes I^A \right) \right].$$

Taking the transpose on E_0, this expression can be rewritten as

$$M^{AB_0} = \mathrm{Tr}_{E_0} \left[\left(\varphi^{E_0 B_0} \otimes I^A \right) \left(\left(J_\Gamma^{E_0 A} \right)^{\mathrm{T}_{E_0}} \otimes I^{B_0} \right) \right].$$

Now rename E_0 as R_0, and define $J_\mathcal{N}^{R_0 A} := J_\Gamma^{R_0 A}$, and $\rho^{R_0 B_0} := \varphi^{R_0 B_0}$. We find that M^{AB_0} can be written in the form of Eq. (B.5). $\qquad \square$

This means that, once we require M^{AB_0} to be positive semi-definite with marginal $M^{A_0 B_0} = I^{A_0} \otimes \rho^{B_0}$, for some density matrix ρ^{B_0}, this automatically implies that M^{AB_0} has the special form of Eq. (B.5). Consequently, we can express the requirement of complete CPTNI preservation in the Choi form as follows: $\Theta^{A \to B}$ is complete CPTNI-preserving if and only if $\mathbf{J}_\Theta^{AB} \geq 0$ and $\mathrm{Tr}\left[\mathbf{J}_\Theta^{AB_0} \left(M^{AB_0} \right)^{\mathrm{T}} \right] \leq 1$ for every positive semi-definite M^{AB_0} with marginal $M^{A_0 B_0} = I^{A_0} \otimes \rho^{B_0}$, where $\rho^{B_0} \in \mathfrak{D}\left(\mathcal{H}^{B_0} \right)$. This is Eq. (4.2) in the main article. In particular, $\Theta^{A \to B}$ is a superchannel, which is a completely CPTP-preserving supermap if and only if $\mathrm{Tr}\left[\mathbf{J}_\Theta^{AB_0} \left(M^{AB_0} \right)^{\mathrm{T}} \right] = 1$ for every M^{AB_0} as above.

Note that, among these M^{AB_0}'s we can find matrices of the form $J_\mathcal{N}^A \otimes \rho^{B_0}$, where $\mathcal{N}^A$ is a CPTP map. These matrices are those used to check the CPTNI preservation condition (cf. Eq. (4.1) in the main article). Indeed, $J_\mathcal{N}^A \otimes \rho^{B_0} \geq 0$, and the marginal is:

$$\mathrm{Tr}_{A_1} \left[J_\mathcal{N}^A \otimes \rho^{B_0} \right] = \mathrm{Tr}_{A_1} \left[J_\mathcal{N}^A \right] \otimes \rho^{B_0} = I^{A_0} \otimes \rho^{B_0},$$

because $J_\mathcal{N}^A$ is the Choi matrix of a CPTP map (see Appendix A). Therefore, as it must be, we recover in the Choi picture that CPTNI preservation is not stronger than complete CPTNI preservation. In fact, it is strictly weaker, as shown in Appendix C.

Appendix C: A supermap that is CPTNI-preserving, but *not* completely CPTNI-preserving

In this appendix we present the concrete counterexample of a supermap $\Theta^{A \to B}$ that is CPTNI-preserving, but *not completely* CPTNI-preserving. In this construction we take $|A_0| = |A_1| = |B_0| = 2$. Consider a supermap $\Theta^{A \to B}$ that has a Choi matrix with marginal $\mathbf{J}_\Theta^{AB_0} = I^{A_0} \otimes \psi_-^{A_1 B_0}$, where $\psi_-^{A_1 B_0} = |\psi_-\rangle \langle \psi_-|^{A_1 B_0}$, and $|\psi_-\rangle^{A_1 B_0} = \frac{1}{\sqrt{2}} \left(|01\rangle^{A_1 B_0} - |10\rangle^{A_1 B_0} \right)$ is the singlet state. Given this marginal, a possible Choi matrix of the supermap $\Theta^{A \to B}$ is $\mathbf{J}_\Theta^{AB} = I^{A_0} \otimes \psi_-^{A_1 B_0} \otimes u^{B_1}$, where u^{B_1} is the maximally mixed state of B_1. Now we will prove that this supermap is CPTNI-preserving, but *not completely* CPTNI-preserving.

To this end, we first show that $\mathbf{J}_\Theta^{AB}$ satisfies Eq. (4.1) in the main article. If $\mathcal{N}^A$ is a CPTP map and ρ^{B_0} is a density matrix, we have

$$\mathrm{Tr}\left[\mathbf{J}_\Theta^{AB_0} \left(J_\mathcal{N}^A \otimes \rho^{B_0} \right)^{\mathrm{T}} \right] = \mathrm{Tr}\left[\left(I^{A_0} \otimes \psi_-^{A_1 B_0} \right) \left(J_\mathcal{N}^A \otimes \rho^{B_0} \right)^{\mathrm{T}} \right].$$

Now we express $\psi_-^{A_1 B_0}$ in terms of the super-normalized maximally entangled state $\phi_+^{A_1 B_0}$:

$$\psi_-^{A_1 B_0} = \frac{1}{2} \left(I^{A_1} \otimes Y^{B_0} \right) \phi_+^{A_1 B_0} \left(I^{A_1} \otimes Y^{B_0} \right), \tag{C.1}$$

where Y^{B_0} is the Pauli Y matrix. Then:

$$
\begin{aligned}
\mathrm{Tr}\left[\mathbf{J}_\Theta^{AB_0}\left(J_\mathcal{N}^A\otimes\rho^{B_0}\right)^\mathrm{T}\right] &= \frac{1}{2}\mathrm{Tr}\left[\left(I^{A_0}\otimes\left(I^{A_1}\otimes Y^{B_0}\right)\phi_+^{A_1B_0}\left(I^{A_1}\otimes Y^{B_0}\right)\right)\left(J_\mathcal{N}^A\otimes\rho^{B_0}\right)^\mathrm{T}\right] \\
&= \frac{1}{2}\mathrm{Tr}_{A_1B_0}\left\{\mathrm{Tr}_{A_0}\left[\left(I^{A_0}\otimes\left(I^{A_1}\otimes Y^{B_0}\right)\phi_+^{A_1B_0}\left(I^{A_1}\otimes Y^{B_0}\right)\right)\left(J_\mathcal{N}^A\otimes\rho^{B_0}\right)^\mathrm{T}\right]\right\} \\
&= \frac{1}{2}\mathrm{Tr}_{A_1B_0}\left[\phi_+^{A_1B_0}\left(\left(J_\mathcal{N}^{A_1}\right)^\mathrm{T}\otimes Y^{B_0}\left(\rho^{B_0}\right)^\mathrm{T}Y^{B_0}\right)\right],
\end{aligned}
$$

using the cyclic property of the trace. Now let us expand $\phi_+^{A_1B_0}$.

$$
\begin{aligned}
\frac{1}{2}\mathrm{Tr}\left[\phi_+^{A_1B_0}\left(\left(J_\mathcal{N}^{A_1}\right)^\mathrm{T}\otimes Y^{B_0}\left(\rho^{B_0}\right)^\mathrm{T}Y^{B_0}\right)\right] &= \frac{1}{2}\mathrm{Tr}\left[\sum_{x,y=1}^2 |xx\rangle\langle yy|^{A_1B_0}\left(\left(J_\mathcal{N}^{A_1}\right)^\mathrm{T}\otimes Y^{B_0}\left(\rho^{B_0}\right)^\mathrm{T}Y^{B_0}\right)\right] \\
&= \frac{1}{2}\mathrm{Tr}\left[\sum_{x,y=1}^2\left\langle y\left|\left(J_\mathcal{N}^{A_1}\right)^\mathrm{T}\right|x\right\rangle^{A_1}|x\rangle\langle y|^{B_0}Y^{B_0}\left(\rho^{B_0}\right)^\mathrm{T}Y^{B_0}\right] \\
&= \frac{1}{2}\mathrm{Tr}\left[\sum_{x,y=1}^2\left\langle x\left|J_\mathcal{N}^{A_1}\right|y\right\rangle^{A_1}|x\rangle\langle y|^{B_0}Y^{B_0}\left(\rho^{B_0}\right)^\mathrm{T}Y^{B_0}\right]. \qquad \text{(C.2)}
\end{aligned}
$$

Here the expression $\sum_{x,y=1}^2\left\langle x\left|J_\mathcal{N}^{A_1}\right|y\right\rangle^{A_1}|x\rangle\langle y|^{B_0}$ means considering $\mathcal{N}^A$ with its output system transformed from A_1 to B_0. With this simplification, Eq. (C.2) reads

$$
\mathrm{Tr}\left[\mathbf{J}_\Theta^{AB_0}\left(J_\mathcal{N}^A\otimes\rho^{B_0}\right)^\mathrm{T}\right] = \frac{1}{2}\mathrm{Tr}\left[J_\mathcal{N}^{B_0}Y^{B_0}\left(\rho^{B_0}\right)^\mathrm{T}Y^{B_0}\right].
$$

Now, both $\frac{1}{2}J_\mathcal{N}^{B_0}$ and $Y^{B_0}\left(\rho^{B_0}\right)^\mathrm{T}Y^{B_0}$ are density operators, therefore

$$
\mathrm{Tr}\left[\mathbf{J}_\Theta^{AB_0}\left(J_\mathcal{N}^A\otimes\rho^{B_0}\right)^\mathrm{T}\right] = \mathrm{Tr}\left[\left(\frac{1}{2}J_\mathcal{N}^{B_0}\right)\left(Y^{B_0}\left(\rho^{B_0}\right)^\mathrm{T}Y^{B_0}\right)\right] \le 1.
$$

Hence $\mathbf{J}_\Theta^{AB_0}$ satisfies Eq. (4.1) in the main article; therefore $\Theta^{A\to B}$ is a CPTNI-preserving supermap.

Now we show that $\Theta^{A\to B}$ violates Eq. (4.2) in the main article. To this end, let us take $M^{AB_0} = \left(\mathbf{J}_\Theta^{AB_0}\right)^\mathrm{T}$. This choice of M^{AB_0} complies with the two requests on M^{AB_0} in Eq. (4.2) in the main article. Since $\mathbf{J}_\Theta^{AB_0} = I^{A_0}\otimes\psi_-^{A_1B_0}$, $\left(\mathbf{J}_\Theta^{AB_0}\right)^\mathrm{T}$ is positive semi-definite; and its marginal

$$
M^{A_0B_0} = \mathrm{Tr}_{A_1}\left[\left(\mathbf{J}_\Theta^{AB_0}\right)^\mathrm{T}\right] = \left(\mathrm{Tr}_{A_1}\left[\mathbf{J}_\Theta^{AB_0}\right]\right)^\mathrm{T} = \left(I^{A_0}\otimes u^{B_0}\right)^\mathrm{T} = I^{A_0}\otimes u^{B_0}
$$

is of the form $I^{A_0}\otimes\rho^{B_0}$, with ρ^{B_0} density matrix. Then:

$$
\begin{aligned}
\mathrm{Tr}\left[\mathbf{J}_\Theta^{AB_0}\left(M^{AB_0}\right)^\mathrm{T}\right] &= \mathrm{Tr}\left[\left(I^{A_0}\otimes\psi_-^{A_1B_0}\right)\left(I^{A_0}\otimes\psi_-^{A_1B_0}\right)\right] \\
&= \mathrm{Tr}\left[I^{A_0}\otimes\left(\psi_-^{A_1B_0}\right)^2\right] \\
&= \mathrm{Tr}_{A_1B_0}\left\{\mathrm{Tr}_{A_0}\left[I^{A_0}\otimes\psi_-^{A_1B_0}\right]\right\} \\
&= 2\mathrm{Tr}\left[\psi_-^{A_1B_0}\right] \\
&= 2 > 1.
\end{aligned}
$$

This is in contrast with Eq. (4.2) in the main article, therefore the supermap $\Theta^{A\to B}$ is *not* a *completely* CPTNI-preserving supermap, despite being CPTNI-preserving.

We conclude this appendix by reconstructing $\Theta^{A\to B}$ from its Choi matrix $\mathbf{J}_\Theta^{AB} = I^{A_0}\otimes\psi_-^{A_1B_0}\otimes u^{B_1}$. By Eqs. (B.1)

and (B.2), we have, if $\mathcal{E}^A$ is a generic CP map,

$$
\begin{aligned}
\Theta^{A\to B}\left[\mathcal{E}^A\right]\left(\rho^{B_0}\right) &= \mathrm{Tr}_{AB_0}\left[\mathbf{J}_\Theta^{AB}\left(J_\mathcal{E}^A\otimes\rho^{B_0}\otimes I^{B_1}\right)^{\mathrm{T}}\right] \\
&= \mathrm{Tr}_{AB_0}\left[\left(I^{A_0}\otimes\psi_-^{A_1B_0}\right)\left(J_\mathcal{E}^A\otimes\rho^{B_0}\right)^{\mathrm{T}}\right]u^{B_1} \\
&= \mathrm{Tr}_{A_1B_0}\left\{\mathrm{Tr}_{A_0}\left[\left(I^{A_0}\otimes\psi_-^{A_1B_0}\right)\left(J_\mathcal{E}^A\otimes\rho^{B_0}\right)^{\mathrm{T}}\right]\right\}u^{B_1} \\
&= \mathrm{Tr}\left[\psi_-^{A_1B_0}\left(J_\mathcal{E}^{A_1}\otimes\rho^{B_0}\right)^{\mathrm{T}}\right]u^{B_1}.
\end{aligned}
$$

Recalling Eq. (C.1), we get

$$
\Theta^{A\to B}\left[\mathcal{E}^A\right]\left(\rho^{B_0}\right) = \frac{1}{2}\mathrm{Tr}\left[\phi_+^{A_1B_0}\left(\left(J_\mathcal{E}^{A_1}\right)^{\mathrm{T}}\otimes Y^{B_0}\left(\rho^{B_0}\right)^{\mathrm{T}}Y^{B_0}\right)\right]u^{B_1},
$$

and using an argument similar to the one in Eq. (C.2), we finally obtain

$$
\Theta^{A\to B}\left[\mathcal{E}^A\right]\left(\rho^{B_0}\right) = \frac{1}{2}\mathrm{Tr}\left[J_\mathcal{E}^{B_0}Y^{B_0}\left(\rho^{B_0}\right)^{\mathrm{T}}Y^{B_0}\right]u^{B_1}. \tag{C.3}
$$

By Eq. (B.1), $\mathcal{E}^{A_0\to B_0}\left(u^{A_0}\right) = \frac{1}{2}\mathrm{Tr}_{A_0}\left[J_\mathcal{E}^{A_0B_0}I^{A_0B_0}\right] = \frac{1}{2}J_\mathcal{E}^{B_0}$. An equivalent form of Eq. (C.3) is, therefore,

$$
\Theta^{A\to B}\left[\mathcal{E}^A\right]\left(\rho^{B_0}\right) = \mathrm{Tr}\left[\mathcal{E}^{A_0\to B_0}\left(u^{A_0}\right)Y^{B_0}\left(\rho^{B_0}\right)^{\mathrm{T}}Y^{B_0}\right]u^{B_1}.
$$

This is exactly Eq. (2.4) in the main article.

Appendix D: The main result

In this appendix we prove the main result of this article, namely that a supermap can be part of a super-instrument if and only if it is completely CPTNI-preserving. To this end, it is useful to consider the SDP (4.3) in the main article, reported here for the reader's convenience.

$$
\begin{aligned}
\text{Find}\quad &\alpha = \max_M \mathrm{Tr}\left[\mathbf{J}_\Theta^{AB_0}\left(M^{AB_0}\right)^{\mathrm{T}}\right] \\
\text{Subject to:}\quad &M^{AB_0}\geq 0 \\
&M^{A_0B_0} = I^{A_0}\otimes\rho^{B_0}.
\end{aligned}
$$

Theorem D.1. *Suppose $\Theta^{A\to B}$ is CPTNI-preserving supermap. Then there exists another CPTNI-preserving supermap $\Theta'^{A\to B}$ such that $\Theta^{A\to B}+\Theta'^{A\to B}$ is a superchannel if and only if $\Theta^{A\to B}$ is completely CPTNI-preserving.*

Proof. First we will show sufficiency, namely that any completely CPTNI-preserving supermap $\Theta^{A\to B}$ can be completed to a superchannel. Following [69], let us write the SDP (4.3) in the main article in a different form. To do so, consider the linear map $\mathcal{L}:\mathfrak{B}_h\left(\mathcal{H}^{AB_0}\right)\to\mathbb{R}\oplus\mathfrak{B}_h\left(\mathcal{H}^{A_0B_0}\right)$, defined as

$$
\mathcal{L}\left(M^{AB_0}\right) = \left(\mathrm{Tr}\left[M^{AB_0}\right], M^{A_0B_0}-u^{A_0}\otimes M^{B_0}\right),
$$

for every hermitian matrix M^{AB_0}. We are working with with positive semi-definite matrices M^{AB_0} with marginal $M^{A_0B_0} = I^{A_0}\otimes\rho^{B_0}$, where $\rho^{B_0}\in\mathfrak{D}\left(\mathcal{H}^{B_0}\right)$, whence

$$
\mathrm{Tr}\left[M^{AB_0}\right] = \mathrm{Tr}_{A_0B_0}\left\{\mathrm{Tr}_{A_1}\left[M^{AB_0}\right]\right\} = \mathrm{Tr}\left[M^{A_0B_0}\right] = \mathrm{Tr}\left[I^{A_0}\otimes\rho^{B_0}\right] = |A_0|.
$$

In addition,

$$
M^{B_0} = \mathrm{Tr}_A\left[M^{AB_0}\right] = \mathrm{Tr}_{A_0}\left[M^{A_0B_0}\right] = \mathrm{Tr}_{A_0}\left[I^{A_0}\otimes\rho^{B_0}\right] = |A_0|\rho^{B_0}.
$$

Using $\mathcal{L}$, we can replace the condition $M^{A_0B_0} = I^{A_0}\otimes\rho^{B_0}$ with $\mathcal{L}\left(M^{AB_0}\right)-\left(|A_0|,0^{A_0B_0}\right) = \left(0,0^{A_0B_0}\right)$. Rewriting the SDP (4.3) in the main article in terms of $\mathcal{L}$, one obtains:

$$
\begin{aligned}
\text{Find}\quad &\alpha = \max_M \mathrm{Tr}\left[\mathbf{J}_\Theta^{AB_0}\left(M^{AB_0}\right)^{\mathrm{T}}\right] \\
\text{Subject to:}\quad &\mathcal{L}\left(M^{AB_0}\right)-\left(|A_0|,0^{A_0B_0}\right) = \left(0,0^{A_0B_0}\right) \\
&M^{AB_0}\geq 0.
\end{aligned}
$$

We can now construct the associated dual problem as follows. The dual map of $\mathcal{L}$ is $\mathcal{L}^* : \mathbb{R} \oplus \mathfrak{B}_h \left(\mathcal{H}^{A_0 B_0} \right) \to \mathfrak{B}_h \left(\mathcal{H}^{A B_0} \right)$ such that

$$\mathcal{L}^* \left(r, \sigma^{A_0 B_0} \right) = \left(r I^{A_0 B_0} + \sigma^{A_0 B_0} - u^{A_0} \otimes \sigma^{B_0} \right) \otimes I^{A_1},$$

where $\left(r, \sigma^{A_0 B_0} \right) \in \mathbb{R} \oplus \mathfrak{B}_h \left(\mathcal{H}^{A_0 B_0} \right)$. The dual problem is then:

$$\begin{aligned}
\text{Find} \quad & \beta = \min \left\langle \left(r, \sigma^{A_0 B_0} \right), \left(|A_0|, 0 \right) \right\rangle \\
\text{Subject to:} \quad & \left(r I^{A_0 B_0} + \sigma^{A_0 B_0} - u^{A_0} \otimes \sigma^{B_0} \right) \otimes I^{A_1} - \mathbf{J}_\Theta^{A B_0} \geq 0 \\
& r \in \mathbb{R} \\
& \sigma^{A_0 B_0} \in \mathfrak{B}_h \left(\mathcal{H}^{A_0 B_0} \right),
\end{aligned}$$

where the inner product $\left\langle \left(r, \sigma^{A_0 B_0} \right), \left(s, \tau^{A_0 B_0} \right) \right\rangle$ is defined as

$$\left\langle \left(r, \sigma^{A_0 B_0} \right), \left(s, \tau^{A_0 B_0} \right) \right\rangle = rs + \mathrm{Tr} \left[\sigma^{A_0 B_0} \tau^{A_0 B_0} \right].$$

With this in mind, the dual problem simplifies to:

$$\begin{aligned}
\text{Find} \quad & \beta = |A_0| \min r \\
\text{Subject to:} \quad & \left(r I^{A_0 B_0} + \sigma^{A_0 B_0} - u^{A_0} \otimes \sigma^{B_0} \right) \otimes I^{A_1} \geq \mathbf{J}_\Theta^{A B_0} \\
& r \in \mathbb{R} \\
& \sigma^{A_0 B_0} \in \mathfrak{B}_h \left(\mathcal{H}^{A_0 B_0} \right).
\end{aligned} \tag{D.1}$$

Notice that the matrix $r I^{A_0 B_0} + \sigma^{A_0 B_0} - u^{A_0} \otimes \sigma^{B_0}$ must be positive semi-definite, otherwise the first constraint could not be satisfied. In particular this implies $r \geq 0$. Indeed, if $r < 0$, for some $\sigma^{A_0 B_0}$ the matrix $r I^{A_0 B_0} + \sigma^{A_0 B_0} - u^{A_0} \otimes \sigma^{B_0}$ would have negative eigenvalues. Factoring $r |A_0|$ out of the first term of the constraint in Eq. (D.1), we get

$$\left(r I^{A_0 B_0} + \sigma^{A_0 B_0} - u^{A_0} \otimes \sigma^{B_0} \right) \otimes I^{A_1} = r |A_0| \left(u^{A_0} \otimes I^{B_0} + \sigma'^{A_0 B_0} - u^{A_0} \otimes \sigma'^{B_0} \right) \otimes I^{A_1},$$

where $\sigma'^{A_0 B_0} := \frac{1}{r |A_0|} \sigma^{A_0 B_0}$ if $r \neq 0$. Note that this does not alter the constraint on the dual SDP, so we can forget the primes, and rewrite Eq. (D.1) as:

$$\begin{aligned}
\text{Find} \quad & \beta = |A_0| \min r \\
\text{Subject to:} \quad & r |A_0| \left(u^{A_0} \otimes I^{B_0} + \sigma^{A_0 B_0} - u^{A_0} \otimes \sigma^{B_0} \right) \otimes I^{A_1} \geq \mathbf{J}_\Theta^{A B_0} \\
& r \geq 0 \\
& \sigma^{A_0 B_0} \in \mathfrak{B}_h \left(\mathcal{H}^{A_0 B_0} \right).
\end{aligned}$$

In particular, this implies that $u^{A_0} \otimes I^{B_0} + \sigma^{A_0 B_0} - u^{A_0} \otimes \sigma^{B_0} \geq 0$. Now let us define

$$\mathbf{J}_\Phi^{A B_0} := \left(u^{A_0} \otimes I^{B_0} + \sigma^{A_0 B_0} - u^{A_0} \otimes \sigma^{B_0} \right) \otimes I^{A_1}. \tag{D.2}$$

Note that $\mathbf{J}_\Phi^{A B_0} = \mathbf{J}_\Phi^{A_0 B_0} \otimes u^{A_1}$ because

$$\mathbf{J}_\Phi^{A_0 B_0} = \mathrm{Tr}_{A_1} \left[\mathbf{J}_\Phi^{A B_0} \right] = |A_1| \left(u^{A_0} \otimes I^{B_0} + \sigma^{A_0 B_0} - u^{A_0} \otimes \sigma^{B_0} \right).$$

Moreover,

$$\mathbf{J}_\Phi^{A_1 B_0} = \mathrm{Tr}_{A_0} \left[\mathbf{J}_\Phi^{A B_0} \right] = \left(I^{B_0} + \sigma^{B_0} - \sigma^{B_0} \right) \otimes I^{A_1} = I^{A_1 B_0}.$$

Since $\mathbf{J}_\Phi^{A_0 B_0} \geq 0$, by Appendix B 1 $\mathbf{J}_\Phi^{A B_0}$ is the marginal Choi matrix of a superchannel $\Phi^{A \to B}$. Eq. (D.2) can be taken as the definition of the marginal $\mathbf{J}_\Phi^{A B_0}$ of the Choi matrix of *any* superchannel. This is because any such marginal $\mathbf{J}_\Phi^{A B_0}$ can be written as in Eq. (D.2) for some hermitian matrix $\sigma^{A_0 B_0}$: it is enough to take $\sigma^{A_0 B_0}$ to be $\frac{1}{|A_1|} \mathbf{J}_\Phi^{A_0 B_0}$.

Indeed, substituting $\sigma^{A_0 B_0} = \frac{1}{|A_1|} \mathbf{J}_\Phi^{A_0 B_0}$ in the right-hand side of Eq. (D.2) yields:

$$
|A_1| \left(u^{A_0} \otimes I^{B_0} + \frac{1}{|A_1|} \mathbf{J}_\Phi^{A_0 B_0} - \frac{1}{|A_1|} u^{A_0} \otimes \mathbf{J}_\Phi^{B_0} \right) \otimes u^{A_1} = \left(|A_1| u^{A_0} \otimes I^{B_0} + \mathbf{J}_\Phi^{A_0 B_0} - u^{A_0} \otimes \mathbf{J}_\Phi^{B_0} \right) \otimes u^{A_1}
$$

$$
= \left(|A_1| u^{A_0} \otimes I^{B_0} + \mathbf{J}_\Phi^{A_0 B_0} - u^{A_0} \otimes \mathrm{Tr}_{AB_1} \left[\mathbf{J}_\Phi^{AB} \right] \right) \otimes u^{A_1}
$$

$$
= \left(|A_1| u^{A_0} \otimes I^{B_0} + \mathbf{J}_\Phi^{A_0 B_0} - u^{A_0} \otimes \mathrm{Tr}_{A_1} \left\{ \mathrm{Tr}_{A_0 B_1} \left[\mathbf{J}_\Phi^{AB} \right] \right\} \right) \otimes u^{A_1}
$$

$$
= \left(|A_1| u^{A_0} \otimes I^{B_0} + \mathbf{J}_\Phi^{A_0 B_0} - u^{A_0} \otimes \mathrm{Tr}_{A_1} \left[\mathbf{J}_\Phi^{A_1 B_0} \right] \right) \otimes u^{A_1}
$$

$$
= \left(|A_1| u^{A_0} \otimes I^{B_0} + \mathbf{J}_\Phi^{A_0 B_0} - u^{A_0} \otimes \mathrm{Tr}_{A_1} \left[I^{A_1 B_0} \right] \right) \otimes u^{A_1}
$$

$$
= \left(|A_1| u^{A_0} \otimes I^{B_0} + \mathbf{J}_\Phi^{A_0 B_0} - |A_1| u^{A_0} \otimes I^{B_0} \right) \otimes u^{A_1}
$$

$$
= \mathbf{J}_\Phi^{A_0 B_0} \otimes u^{A_1}.
$$

Therefore, in the light of these remarks, the dual SDP can equivalently be formulated in the following terms:

$$
\text{Find} \quad \beta = |A_0| \min r
$$
$$
\text{Subject to:} \quad r |A_0| \mathbf{J}_\Phi^{A_0 B_0} \otimes u^{A_1} \geq \mathbf{J}_\Theta^{AB_0}
$$
$$
\mathbf{J}_\Phi^{A_0 B_0} \geq 0
$$
$$
\mathbf{J}_\Phi^{A_1 B_0} = I^{A_1 B_0}
$$
$$
r \geq 0.
$$

Strong duality states that the primal and dual problem have the same optimal solution, therefore $\alpha = \beta$. Since $\Theta^{A \to B}$ is completely CPTNI-preserving, $\alpha = \max_M \mathrm{Tr} \left[\mathbf{J}_\Theta^{AB_0} \left(M^{AB_0} \right)^{\mathrm{T}} \right] \leq 1$. Hence $\beta \leq 1$. Clearly taking $r |A_0| = \beta$ satisfies the constraint $r |A_0| \mathbf{J}_\Phi^{A_0 B_0} \otimes u^{A_1} \geq \mathbf{J}_\Theta^{AB_0}$, and we have

$$
\mathbf{J}_\Phi^{A_0 B_0} \otimes u^{A_1} \geq \beta \mathbf{J}_\Phi^{A_0 B_0} \otimes u^{A_1} \geq \mathbf{J}_\Theta^{AB_0},
$$

because $\beta \leq 1$. Now define $\Theta'^{A \to B}$ to be a new supermap such that $\mathbf{J}_{\Theta'}^{AB_0} := \mathbf{J}_\Phi^{A_0 B_0} \otimes u^{A_1} - \mathbf{J}_\Theta^{AB_0}$. By construction $\mathbf{J}_{\Theta'}^{AB_0} \geq 0$; and by substituting $\mathbf{J}_{\Theta'}^{AB_0}$ into the left-hand side of Eq. (4.1) in the main article one obtains:

$$
\mathrm{Tr} \left[\mathbf{J}_{\Theta'}^{AB_0} \left(J_\mathcal{N}^A \otimes \rho^{B_0} \right)^{\mathrm{T}} \right] = \mathrm{Tr} \left[\left(\mathbf{J}_\Phi^{AB_0} - \mathbf{J}_\Theta^{AB_0} \right) \left(J_\mathcal{N}^A \otimes \rho^{B_0} \right)^{\mathrm{T}} \right]
$$

$$
= \mathrm{Tr} \left[\mathbf{J}_\Phi^{AB_0} \left(J_\mathcal{N}^A \otimes \rho^{B_0} \right)^{\mathrm{T}} \right] - \mathrm{Tr} \left[\mathbf{J}_\Theta^{AB_0} \left(J_\mathcal{N}^A \otimes \rho^{B_0} \right)^{\mathrm{T}} \right]
$$

$$
= 1 - \mathrm{Tr} \left[\mathbf{J}_\Theta^{AB_0} \left(J_\mathcal{N}^A \otimes \rho^{B_0} \right)^{\mathrm{T}} \right],
$$

where we have used the fact that $\Phi^{A \to B}$ is a superchannel (see Appendix B 1). Now, $\mathrm{Tr} \left[\mathbf{J}_\Theta^{AB_0} \left(J_\mathcal{N}^A \otimes \rho^{B_0} \right)^{\mathrm{T}} \right] \geq 0$ because $\Theta^{A \to B}$ is CPP. Therefore $\mathrm{Tr} \left[\mathbf{J}_{\Theta'}^{AB_0} \left(J_\mathcal{N}^A \otimes \rho^{B_0} \right)^{\mathrm{T}} \right] \leq 1$ for every $J_\mathcal{N}^A \otimes \rho^{B_0}$, thus $\Theta'^{A \to B}$ is CPTNI-preserving.

To conclude the proof, let us prove necessity. Assume that $\Theta^{A \to B}$ is a CPTNI-preserving supermap such that $\Phi^{A \to B} = \Theta^{A \to B} + \Theta'^{A \to B}$ is a superchannel, where $\Theta'^{A \to B}$ is another CPTNI-preserving supermap. We will prove that $\Theta^{A \to B}$ must be *completely* CPTNI-preserving. In the Choi picture we have

$$
\mathbf{J}_\Theta^{AB_0} + \mathbf{J}_{\Theta'}^{AB_0} = \mathbf{J}_\Phi^{AB_0}. \tag{D.3}
$$

Let us multiply both sides of Eq. (D.3) by the transpose of any matrix $M^{AB_0} \geq 0$ with marginal $M^{A_0 B_0} = I^{A_0} \otimes \rho^{B_0}$, $\rho^{B_0} \in \mathfrak{D} \left(\mathcal{H}^{B_0} \right)$, and then take the trace.

$$
\mathrm{Tr} \left[\mathbf{J}_\Theta^{AB_0} \left(M^{AB_0} \right)^{\mathrm{T}} \right] + \mathrm{Tr} \left[\mathbf{J}_{\Theta'}^{AB_0} \left(M^{AB_0} \right)^{\mathrm{T}} \right] = \mathrm{Tr} \left[\mathbf{J}_\Phi^{AB_0} \left(M^{AB_0} \right)^{\mathrm{T}} \right] \tag{D.4}
$$

By the results in Appendix B 2, the right-hand side is 1 because $\Phi^{A \to B}$ is a superchannel. Thus Eq. (D.4) becomes

$$
\mathrm{Tr} \left[\mathbf{J}_\Theta^{AB_0} \left(M^{AB_0} \right)^{\mathrm{T}} \right] + \mathrm{Tr} \left[\mathbf{J}_{\Theta'}^{AB_0} \left(M^{AB_0} \right)^{\mathrm{T}} \right] = 1,
$$

which implies $\mathrm{Tr} \left[\mathbf{J}_\Theta^{AB_0} \left(M^{AB_0} \right)^{\mathrm{T}} \right] \leq 1$ for all M^{AB_0} because $\Theta^{A \to B}$ is CPP. Therefore $\Theta^{A \to B}$ satisfies Eq. (4.2) in the main article, which means that it is completely CPTNI-preserving. This concludes the proof. $\square$

Applying the statement of this theorem to $\Theta'^{A \to B}$, we get that $\Theta'^{A \to B}$ is completely CPTNI-preserving too.

Appendix E: Quantum super-instruments

In this appendix we re-derive one of the results of [14], but in a different way. This new proof is based on our main result: every completely CPTNI-preserving supermap can be completed to a superchannel. Specifically, we show that each completely CPTNI-preserving supermap $\Theta_x^{A \to B}$ in a super-measurement $\left\{\Theta_x^{A \to B}\right\}$ can be expressed in terms of a CPTP pre-processing channel, independent of x, and a CPTNI post-processing map, as depicted in Fig. 4.

Proposition E.1. *The Choi matrix $\mathbf{J}_{\Theta_x}^{AB}$ of each completely CPTNI-preserving supermap $\Theta_x^{A \to B}$ in a super-measurement $\left\{\Theta_x^{A \to B}\right\}_{x \in X}$ can be written in terms of a common CPTP pre-processing map $\Gamma_{\mathrm{pre}}^{\widetilde{B}_0 \to A_0 E_0}$, and a CPTNI post-processing map $\Gamma_{\mathrm{post}_x}^{\widetilde{A}_1 E_0 \to B_1}$ as*

$$\mathbf{J}_{\Theta_x}^{AB} = \left(\mathcal{I}^{AB_0} \otimes \Gamma_{\mathrm{post}_x}^{\widetilde{A}_1 E_0 \to B_1}\right) \circ \left(\mathcal{I}^{A_1 \widetilde{A}_1 B_0} \otimes \Gamma_{\mathrm{pre}}^{\widetilde{B}_0 \to A_0 E_0}\right) \left(\phi_+^{B_0 \widetilde{B}_0} \otimes \phi_+^{A_1 \widetilde{A}_1}\right).$$

Proof. Define $\Theta^{A \to B} := \sum_{x \in X} \Theta_x^{A \to B}$, which we know to be a superchannel. In the Choi picture this is translated into $\mathbf{J}_{\Theta}^{AB} = \sum_x \mathbf{J}_{\Theta_x}^{AB}$. In [38, theorem 1] one of the authors showed that the Choi matrix of a superchannel can be written in terms of its pre-processing $\Gamma_{\mathrm{pre}}^{B_0 \to A_0 E_0}$ and post-processing $\Gamma_{\mathrm{post}}^{A_1 E_0 \to B_1}$ as

$$\mathbf{J}_{\Theta}^{AB} = \left(\mathcal{I}^{AB_0} \otimes \Gamma_{\mathrm{post}}^{\widetilde{A}_1 E_0 \to B_1}\right) \left(\psi^{A_0 B_0 E_0} \otimes \phi_+^{A_1 \widetilde{A}_1}\right),$$

where $\psi^{A_0 B_0 E_0} := \left(\mathcal{I}^{AB_0} \otimes \Gamma_{\mathrm{pre}}^{\widetilde{B}_0 \to A_0 E_0}\right) \left(\phi_+^{B_0 \widetilde{B}_0}\right)$. $\psi^{A_0 B_0 E_0}$ can be shown to be a purification of $\frac{1}{|A_1|}\mathbf{J}_{\Theta}^{A_0 B_0}$ [38]. Now, summing over all outcomes $x \in X$, let us construct the matrix $\sum_{x \in X} |x\rangle \langle x|^{X_1} \otimes \mathbf{J}_{\Theta_x}^{AB}$, where $\left\{|x\rangle^{X_1}\right\}_{x=1}^{|X_1|}$ is an orthonormal basis of $\mathcal{H}^{X_1}$. Let $\varphi^{X_1 ABF_0}$ be a purification of $\sum_x |x\rangle \langle x|^{X_1} \otimes \mathbf{J}_{\Theta_x}^{AB}$. Note that $\varphi^{X_1 ABF_0}$ is a purification of $\mathbf{J}_{\Theta}^{AB}$ too, because

$$\mathrm{Tr}_{X_1 F_0}\left[\varphi^{X_1 ABF_0}\right] = \mathrm{Tr}_{X_1}\left\{\mathrm{Tr}_{F_0}\left[\varphi^{X_1 ABF_0}\right]\right\} = \mathrm{Tr}_{X_1}\left[\sum_x |x\rangle \langle x|^{X_1} \otimes \mathbf{J}_{\Theta_x}^{AB}\right] = \sum_x \mathbf{J}_{\Theta_x}^{AB} = \mathbf{J}_{\Theta}^{AB}.$$

If we take the isometry $\mathcal{V}^{\widetilde{A}_1 E_0 \to B_1 G_0}$ to be a Stinespring dilation of $\Gamma_{\mathrm{post}}^{\widetilde{A}_1 E_0 \to B_1}$, namely $\Gamma_{\mathrm{post}}^{\widetilde{A}_1 E_0 \to B_1} = \mathrm{Tr}_{G_0} \circ \mathcal{V}^{\widetilde{A}_1 E_0 \to B_1 G_0}$, then

$$\chi^{ABG_0} := \left(\mathcal{I}^{AB_0} \otimes \mathcal{V}^{\widetilde{A}_1 E_0 \to B_1 G_0}\right) \left(\psi^{A_0 B_0 E_0} \otimes \phi_+^{A_1 \widetilde{A}_1}\right)$$

is another purification of $\mathbf{J}_{\Theta}^{AB}$. Indeed,

$$\begin{aligned}
\mathrm{Tr}_{G_0}\left[\chi^{ABG_0}\right] &= \mathcal{I}^{AB_0} \otimes \left(\mathrm{Tr}_{G_0} \circ \mathcal{V}^{\widetilde{A}_1 E_0 \to B_1 G_0}\right) \left(\psi^{A_0 B_0 E_0} \otimes \phi_+^{A_1 \widetilde{A}_1}\right) \\
&= \left(\mathcal{I}^{AB_0} \otimes \Gamma_{\mathrm{post}}^{\widetilde{A}_1 E_0 \to B_1}\right) \left(\psi^{A_0 B_0 E_0} \otimes \phi_+^{A_1 \widetilde{A}_1}\right) \\
&= \mathbf{J}_{\Theta}^{AB}.
\end{aligned}$$

Since both $\varphi^{X_1 ABF_0}$ and χ^{ABG_0} are purifications of $\mathbf{J}_{\Theta}^{AB}$, they are related by an isometry channel $\mathcal{U}^{G_0 \to X_1 F_0}$ such that

$$\begin{aligned}
\varphi^{X_1 ABF_0} &= \left(\mathcal{I}^{AB} \otimes \mathcal{U}^{G_0 \to X_1 F_0}\right) \left(\chi^{ABG_0}\right) \\
&= \left(\mathcal{I}^{AB} \otimes \mathcal{U}^{G_0 \to X_1 F_0}\right) \left(\mathcal{I}^{AB_0} \otimes \mathcal{V}^{\widetilde{A}_1 E_0 \to B_1 G_0}\right) \left(\psi^{A_0 B_0 E_0} \otimes \phi_+^{A_1 \widetilde{A}_1}\right) \\
&=: \left(\mathcal{I}^{AB_0} \otimes \mathcal{W}^{\widetilde{A}_1 E_0 \to B_1 X_1 F_0}\right) \left(\psi^{A_0 B_0 E_0} \otimes \phi_+^{A_1 \widetilde{A}_1}\right),
\end{aligned}$$

where we have defined $\mathcal{W}^{\widetilde{A}_1 E_0 \to B_1 X_1 F_0} := \mathcal{U}^{G_0 \to X_1 F_0} \circ \mathcal{V}^{\widetilde{A}_1 E_0 \to B_1 G_0}$, which is another isometry channel, and another Stinespring dilation of $\Gamma_{\mathrm{post}}^{\widetilde{A}_1 E_0 \to B_1}$. Now let us trace out system F_0, recalling that $\mathrm{Tr}_{F_0}\left[\varphi^{X_1 ABF_0}\right] = \sum_y |y\rangle \langle y|^{X_1} \otimes \mathbf{J}_{\Theta_y}^{AB}$, where we have changed the index from x to y for convenience. We get

$$\sum_y |y\rangle \langle y|^{X_1} \otimes \mathbf{J}_{\Theta_y}^{AB} = \left(\mathcal{I}^{AB_0} \otimes \widetilde{\Gamma}^{\widetilde{A}_1 E_0 \to B_1 X_1}\right) \left(\psi^{A_0 B_0 E_0} \otimes \phi_+^{A_1 \widetilde{A}_1}\right), \tag{E.1}$$

where $\widetilde{\Gamma}^{\widetilde{A}_1 E_0 \to B_1 X_1} := \mathrm{Tr}_{F_0} \circ \mathcal{W}^{\widetilde{A}_1 E_0 \to B_1 X_1 F_0}$ is a CPTP map. To get $\mathbf{J}_{\Theta_x}^{AB}$, we apply the projector $|x\rangle \langle x|^{X_1}$ to both sides of Eq. (E.1), tracing over X_1:

$$\mathbf{J}_{\Theta_x}^{AB} = \mathrm{Tr}_{X_1}\left[|x\rangle \langle x|^{X_1}\left(\mathcal{I}^{AB_0} \otimes \widetilde{\Gamma}^{\widetilde{A}_1 E_0 \to B_1 X_1}\right)\left(\psi^{A_0 B_0 E_0} \otimes \phi_+^{A_1 \widetilde{A}_1}\right)\right]$$

$$= \left[\mathcal{I}^{AB_0} \otimes \left(\mathrm{Tr}_{X_1} |x\rangle \langle x|^{X_1} \circ \widetilde{\Gamma}^{\widetilde{A}_1 E_0 \to B_1 X_1}\right)\right]\left(\psi^{A_0 B_0 E_0} \otimes \phi_+^{A_1 \widetilde{A}_1}\right). \quad (E.2)$$

Now let us define $\Gamma_{\mathrm{post}_x}^{\widetilde{A}_1 E_0 \to B_1} := \mathrm{Tr}_{X_1} |x\rangle \langle x|^{X_1} \circ \widetilde{\Gamma}^{\widetilde{A}_1 E_0 \to B_1 X_1}$, which is a CPTNI map whose action on a density matrix $\rho^{\widetilde{A}_1 E_0}$ is

$$\Gamma_{\mathrm{post}_x}^{\widetilde{A}_1 E_0 \to B_1}\left(\rho^{\widetilde{A}_1 E_0}\right) = \left\langle x\left|\widetilde{\Gamma}^{\widetilde{A}_1 E_0 \to B_1 X_1}\left(\rho^{\widetilde{A}_1 E_0}\right)\right|x\right\rangle^{X_1}.$$

Therefore Eq. (E.2) becomes

$$\mathbf{J}_{\Theta_x}^{AB} = \left(\mathcal{I}^{AB_0} \otimes \Gamma_{\mathrm{post}_x}^{\widetilde{A}_1 E_0 \to B_1}\right)\left(\psi^{A_0 B_0 E_0} \otimes \phi_+^{A_1 \widetilde{A}_1}\right).$$

Recalling $\psi^{A_0 B_0 E_0} = \left(\mathcal{I}^{AB_0} \otimes \Gamma_{\mathrm{pre}}^{\widetilde{B}_0 \to A_0 E_0}\right)\left(\phi_+^{B_0 \widetilde{B}_0}\right)$, where $\Gamma_{\mathrm{pre}}^{\widetilde{B}_0 \to A_0 E_0}$ is the pre-processing of the superchannel $\Theta^{A \to B}$, we get the thesis:

$$\mathbf{J}_{\Theta_x}^{AB} = \left(\mathcal{I}^{AB_0} \otimes \Gamma_{\mathrm{post}_x}^{\widetilde{A}_1 E_0 \to B_1}\right) \circ \left(\mathcal{I}^{A_1 \widetilde{A}_1 B_0} \otimes \Gamma_{\mathrm{pre}}^{\widetilde{B}_0 \to A_0 E_0}\right)\left(\phi_+^{B_0 \widetilde{B}_0} \otimes \phi_+^{A_1 \widetilde{A}_1}\right).$$

$\square$

Therefore we can realize every completely CPTNI-preserving supermap $\Theta_x^{A \to B}$ that is part of a quantum super-instrument as a quantum 1-comb, as in Fig. 4. More precisely we have

$$\Theta_x^{A \to B} = \begin{array}{c} \xrightarrow{B_0} \boxed{\Gamma_{\mathrm{pre}}} \xrightarrow{A_0} \quad \xrightarrow{A_1} \boxed{\Gamma_{\mathrm{post}_x}} \xrightarrow{B_1} \\ E_0 \end{array}, \quad (E.3)$$

where $\Gamma_{\mathrm{pre}}^{B_0 \to A_0 E_0}$ is the CPTP pre-processing of the superchannel $\Theta^{A \to B} = \sum_x \Theta_x^{A \to B}$. The pre-processing of a completely CPTNI-preserving supermap is therefore independent of x and common to all the supermaps in the same quantum super-instrument. In fact, even the post-processing is almost shared by all supermaps in the same super-instrument: it is given by $\Gamma_{\mathrm{post}_x}^{A_1 E_0 \to B_1} = \mathrm{Tr}_{X_1} |x\rangle \langle x|^{X_1} \circ \widetilde{\Gamma}^{A_1 E_0 \to B_1 X_1}$, namely by a reading performed on the classical output X_1 of $\widetilde{\Gamma}^{A_1 E_0 \to B_1 X_1}$. $\widetilde{\Gamma}^{A_1 E_0 \to B_1 X_1}$ depends only on the superchannel $\Theta^{A \to B}$, so it is common to all the supermaps in the same super-instrument. Eq. (E.3) then becomes

$$\Theta_x^{A \to B} = \begin{array}{c} \xrightarrow{B_0} \boxed{\Gamma_{\mathrm{pre}}} \xrightarrow{A_0} \quad \xrightarrow{A_1} \boxed{\widetilde{\Gamma}} \xrightarrow{B_1} \\ E_0 \qquad X_1 \boxed{x} \end{array}.$$

From the proof of proposition E.1 we have

$$\mathrm{Tr}_{X_1} \circ \widetilde{\Gamma}^{A_1 E_0 \to B_1 X_1} = \mathrm{Tr}_{X_1 F_0} \circ \mathcal{W}^{A_1 E_0 \to B_1 X_1 F_0} = \Gamma_{\mathrm{post}}^{A_1 E_0 \to B_1}, \quad (E.4)$$

because $\mathcal{W}^{A_1 E_0 \to B_1 X_1 F_0}$ is a Stinespring dilation of $\Gamma_{\mathrm{post}}^{A_1 E_0 \to B_1}$. Therefore, if we forget the outcome x of the super-measurement, Eq. (E.4) yields

$$\sum_x \Gamma_{\mathrm{post}_x}^{A_1 E_0 \to B_1} = \mathrm{Tr}_{X_1} \circ \widetilde{\Gamma}^{A_1 E_0 \to B_1 X_1} = \Gamma_{\mathrm{post}}^{A_1 E_0 \to B_1},$$

and we recover the post-processing channel $\Gamma_{\mathrm{post}}^{A_1 E_0 \to B_1}$ of $\Theta^{A \to B}$.

Appendix F: OPT interpretation of the result

The theory of quantum supermaps, where generic evolutions of quantum maps are described by supermaps, can be analysed using the framework of operational probabilistic theories (OPTs) [58, 65–67, 70–72], which is a formalism to describe arbitrary physical theories admitting probabilistic processes. OPTs differ from the convex set approach to general probabilistic theories [73–75] in that they take the composition of physical processes and systems as a primitive. Mathematically, this is based on the graphical language of circuits [76–79] and probability theory.

1.   The general framework

OPTs describe the experiments that can be performed on a given set of systems by a given set of physical processes. The framework is based on a primitive notion of composition, whereby every pair of physical systems A and B can be combined into a composite system AB. Physical processes can be connected in sequence or in parallel to build circuits, in the very same way as the corresponding devices are connected in a laboratory to build an experiment; for instance

$$
\begin{array}{c}
\rho \quad \underset{\text{B}}{\overset{\text{A}}{}} \boxed{\mathcal{A}} \underset{}{\overset{\text{A}'}{}} \boxed{\mathcal{A}'} \overset{\text{A}''}{} \boxed{a} \\
\boxed{\mathcal{B}} \overset{\text{B}'}{} \boxed{b}
\end{array}
\tag{F.1}
$$

In this example, A, A′, A″, B, and B′ are *systems*, ρ is a bipartite *state*, $\mathcal{A}$, $\mathcal{A}'$ and $\mathcal{B}$ are *transformations*, a and b are *effects*. Note that inputs are on the left and outputs on the right.

For generic systems A and B, we denote:

- the set of states of system A by $\mathsf{St}\,(\mathrm{A})$;

- the set of effects on A by $\mathsf{Eff}\,(\mathrm{A})$;

- the set of transformations from A to B by $\mathsf{Transf}\,(\mathrm{A}, \mathrm{B})$;

- the sequential composition of two transformations $\mathcal{A}$ and $\mathcal{B}$ by $\mathcal{B} \circ \mathcal{A}$ (or $\mathcal{B}\mathcal{A}$, for short), with the input of $\mathcal{B}$ matching the output of $\mathcal{A}$;

- the identity transformation on system A by $\mathcal{I}_{\mathrm{A}}$, represented with a plain wire $\overset{\text{A}}{}$;

- the parallel composition (or tensor product) of the transformations $\mathcal{A}$ and $\mathcal{B}$ by $\mathcal{A} \otimes \mathcal{B}$.

Among the list of valid physical systems, every OPT includes the trivial system I, corresponding to the degrees of freedom ignored by theory, and to the lack of input (or output) system. States (resp. effects) are transformations with the trivial system as input (resp. output).

A circuit with no external wires, as in Eq. (F.1), is identified with a real number in the interval $[0, 1]$, interpreted as the probability of the joint occurrence of all the transformations present in the circuit. We will often use the notation $(a|\rho)$ to denote the circuit

$$
(a|\rho) \;\; := \;\; \boxed{\rho} \overset{\text{A}}{} \boxed{a} \;,
$$

and the notation $(b|\mathcal{C}|\rho)$ to mean the circuit

$$
\boxed{\rho} \overset{\text{A}}{} \boxed{\mathcal{C}} \overset{\text{B}}{} \boxed{b} \;.
$$

Let us clarify these concepts in quantum theory.

Example F.1. In quantum theory, we associate a Hilbert space $\mathcal{H}^A$ with every system A. States are positive semi-definite operators ρ with $\mathrm{Tr}\,[\rho] \leq 1$. The reason why we also consider states with trace less than 1 will be explained in example F.3. An effect is, instead, represented by a positive semi-definite operator E, with $E \leq I$, where I is the identity operator. The pairing between states and effects is given by the trace: $(E|\rho) = \mathrm{Tr}\,[E\rho]$.

The fact that some circuits represent real numbers induces a notion of sum for transformations, so that the sets $\mathsf{St}\,(\mathrm{A})$, $\mathsf{Transf}\,(\mathrm{A}, \mathrm{B})$, and $\mathsf{Eff}\,(\mathrm{A})$ become spanning sets of *real* vector spaces. We will denote the vector space of states as $\mathsf{St}_{\mathbb{R}}\,(\mathrm{A})$ and the vector space of transformations as $\mathsf{Transf}_{\mathbb{R}}\,(\mathrm{A}, \mathrm{B})$. Effects become linear functionals on $\mathsf{St}_{\mathbb{R}}\,(\mathrm{A})$, and transformations in $\mathsf{Transf}\,(\mathrm{A}, \mathrm{B})$ are linear transformations from $\mathsf{St}_{\mathbb{R}}\,(\mathrm{A})$ to $\mathsf{St}_{\mathbb{R}}\,(\mathrm{B})$.

If we restrict ourselves to linear combinations of states with non-negative coefficients (conical combinations), we obtain a proper convex cone [58], called the cone of states $\mathsf{St}_{+}\,(\mathrm{A})$. Note that effects take non-negative values on the cone of states. Indeed if $\xi \in \mathsf{St}_{+}\,(\mathrm{A})$, then ξ is a conical combination of some states ρ_i: $\xi = \sum_i \lambda_i \rho_i$, where $\lambda_i \geq 0$ for every i. Therefore when an effect a acts on ξ, we have

$$
(a|\xi) = \sum_i \lambda_i \,(a|\rho_i) \geq 0,
$$

as $\lambda_i \geq 0$, and $0 \leq (a|\rho_i) \leq 1$, because an effect yields a probability when applied to a state.

Example F.2. In quantum theory, $\mathsf{St}_{\mathbb{R}}(A)$ is the vector space of hermitian matrices on $\mathcal{H}^A$, and $\mathsf{St}_+(A)$ is the cone of positive semi-definite matrices.

In general, an experiment in a laboratory can be non-deterministic, i.e. it can result into a set of alternative transformations applied to the input system, heralded by different outcomes, which can (at least in principle) be accessed by an experimenter. General non-deterministic processes are described by *tests*: a test from A to B is a collection of transformations $\{\mathcal{C}_x\}_{x \in X}$ from A to B, where X is the set of outcomes. If A (resp. B) is the trivial system, the test is called a *preparation-test* (resp. *observation-test*). If the set of outcomes X contains a single element, we say that the test is *deterministic*, because only one transformation can occur, and we can predict the outcome of the experiment. We refer to deterministic transformations as *channels*. If we sum over all the transformations in a test we get a deterministic transformation, viz. a channel: $\mathcal{C} := \sum_{x \in X} \mathcal{C}_x$. This is because the sum of all the transformations arising in a test can be viewed as the full coarse-graining over all outcomes [58], resulting in a new, deterministic, test.

Example F.3. In quantum theory, a channel from A_0 to A_1 is a CPTP map from $\mathfrak{B}\left(\mathcal{H}^{A_0}\right)$ to $\mathfrak{B}\left(\mathcal{H}^{A_1}\right)$. A test from A_0 to A_1 is a collection of CPTNI maps from $\mathfrak{B}\left(\mathcal{H}^{A_0}\right)$ to $\mathfrak{B}\left(\mathcal{H}^{A_1}\right)$ summing to a CPTP map. Note that this is consistent with the fact that the sum over all the transformations in a test yields a channel.

Deterministic states are positive semi-definite operators ρ with $\text{Tr}\left[\rho\right] = 1$. A non-deterministic preparation-test is a collection of positive semi-definite operators ρ_i with $\text{Tr}\left[\rho_i\right] < 1$ (non-deterministic states) that sum to a deterministic state ρ. This is essentially a random preparation: a state ρ_i is prepared with a probability given by $\text{Tr}\left[\rho_i\right]$. This is why we consider all positive semi-definite operators ρ with $\text{Tr}\left[\rho\right] \leq 1$ as states.

Observation-tests are POVMs. In quantum theory there is only one deterministic effect: the identity I (more precisely it is the functional $\text{Tr}\left[I\bullet\right]$). This is not a coincidence, but it follows from the fact that quantum theory is a causal theory (see definition F.4).

Among all theories, *causal* theories [58] are particularly important: in these theories, loosely speaking, information cannot come back from the future. They are particularly simple in their structure, and, generally speaking, they are well understood. Causality can also be shown to imply no-signalling in space-like separated systems [58]. The formal statement of the property of causality is as follows.

Axiom F.4 (Causality [58]). *For every state ρ, take two observation-tests $\{a_x\}_{x \in X}$ and $\{b_y\}_{y \in Y}$. One has*

$$\sum_{x \in X} (a_x|\rho) = \sum_{y \in Y} (b_y|\rho).$$

Causality can be equivalently characterized in terms of deterministic effects: an OPT is *causal* if and only if, for every system A, there is a unique deterministic effect u_A [58]. This characterization is very practical to work with.

Example F.5. In quantum theory there is only one deterministic effect, the identity operator (or the trace functional). Hence quantum theory is causal.

Causal theories enjoy an important property: the unique deterministic effect for a composite system AB always factorizes as the parallel composition of the deterministic effects on A and on B. In symbols, $u_{AB} = u_A \otimes u_B$. This is because if u_A and u_B are the deterministic effects of A and B, then $u_A \otimes u_B$ is a deterministic effect on AB. Since the theory is causal, there is a unique deterministic effect on AB, so $u_A \otimes u_B$ is *the* deterministic effect of AB.

Moreover, in causal theories there is a nice characterization of channels: a transformation $\mathcal{C} \in \mathsf{Transf}(A, B)$ is a channel if and only if [58]

$$u_B \mathcal{C} = u_A. \tag{F.2}$$

In quantum theory, since u is the trace, this condition amounts to saying that channels are trace-preserving.

Let us conclude this section by showing how the theory of quantum supermaps fits into the OPT formalism.

Example F.6. In the theory of quantum supermaps, every system A is a pair of input and output quantum systems $A = (A_0, A_1)$; deterministic states are CPTP maps, and non-deterministic ones are CPTNI maps. The cone of states is given by all CP maps. Transformations in this theory are supermaps [14, 16, 38, 56, 57]. As our results show, it is not immediate to pin down the mathematical properties that make a generic linear supermap from A to B physical. We will analyse this issue from the OPT perspective in the next subsection.

Now let us show that the theory of quantum supermaps is *not* causal. Suppose we want to construct a deterministic effect in this theory. According to [14, 15, 19], to this end it is enough to consider a 1-comb made of deterministic quantum operations, which means a circuit fragment of the form
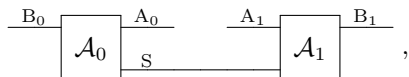
where both $\mathcal{A}_0$ and $\mathcal{A}_1$ are deterministic quantum operations. Since this comb must output a probability, its pre-processing $\mathcal{A}_0$ must be a deterministic bipartite quantum state $\rho \in \mathsf{St}\,(A_0 S)$, and its post-processing $\mathcal{A}_1$ must be a deterministic bipartite quantum effect $u \in \mathsf{Eff}\,(A_1 S)$, for some system S:

$$\left(\rho \begin{array}{c} A_0 \\ S \end{array} \begin{array}{c} A_1 \end{array} u\right).$$

Now recall that in causal theories the deterministic effect of a bipartite system $A_1 S$ factorizes as $u_{A_1} \otimes u_S$, and that u is nothing but the trace (cf. example F.3). Then

$$\left(\rho \begin{array}{c} A_0 \\ S \end{array} \begin{array}{c} A_1 \end{array} u\right) = \left(\rho \begin{array}{c} A_0 \\ S \end{array} \begin{array}{c} A_1 \end{array}\boxed{\mathrm{Tr}}\atop\boxed{\mathrm{Tr}}\right) = \left(\rho' \begin{array}{c} A_0 \end{array}\begin{array}{c} A_1 \end{array}\boxed{\mathrm{Tr}}\right),$$

where $\rho' = \mathrm{Tr}_S\,[\rho]$. In this way, for any choice of $\rho \in \mathfrak{D}\left(\mathcal{H}^{A_0 S}\right)$ we obtain *all* quantum states $\rho' \in \mathfrak{D}\left(\mathcal{H}^{A_0}\right)$. Hence, the generic deterministic effect on system $A = (A_0, A_1)$ of the theory of quantum supermaps is of the form

$$u_\rho = \left(\rho \begin{array}{c} A_0 \end{array}\begin{array}{c} A_1 \end{array}\boxed{\mathrm{Tr}}\right),$$

for any quantum state $\rho \in \mathfrak{D}\left(\mathcal{H}^{A_0}\right)$. This means that there is a whole family of deterministic effects, labelled by quantum states. Therefore, the theory of quantum supermaps is *not* causal, a fact that is confirmed by the presence of signalling bipartite quantum channels [59]. The failure of causality implies here that there are some deterministic effects for a bipartite system $AB = (A_0, A_1)(B_0, B_1)$ that do not factorize. Indeed, if we take an entangled bipartite quantum state $\rho \in \mathfrak{D}\left(\mathcal{H}^{A_0 B_0}\right)$, the associated deterministic effect is

$$u_\rho = \left(\rho \begin{array}{c} A_0 \\ B_0 \end{array} \begin{array}{c} A_1 \\ B_1 \end{array}\boxed{\mathrm{Tr}}\atop\boxed{\mathrm{Tr}}\right), \tag{F.3}$$

which does not factorize. This fact will play an important role in Appendix F 2, and it is ultimately the reason why we need the CPTNI preservation condition in a complete sense.

2. Necessary conditions for physical transformations

In the OPT approach, however we construct a diagram, this represents a physical object: a valid state, a valid transformation, a valid effect. Specializing our analysis to transformations from a system A to a system B, a linear map $\mathcal{A}$ from $\mathsf{St}_{\mathbb{R}}\,(A)$ to $\mathsf{St}_{\mathbb{R}}\,(B)$ is a valid physical transformation only if

$$\left(\rho \begin{array}{c} A \\ S \end{array}\boxed{\mathcal{A}}\begin{array}{c} B \end{array}\right) \tag{F.4}$$

is a valid state of system BS, for every choice of ρ and S. Here we will derive some *necessary* conditions to guarantee this. In particular, if (F.4) is a valid state, for every bipartite effect $E \in \mathsf{Eff}\,(BS)$ we have

$$0 \leq \left(\rho \begin{array}{c} A \\ S \end{array}\boxed{\mathcal{A}}\begin{array}{c} B \end{array} E\right) \leq 1, \tag{F.5}$$

because this is the probability of E occurring on $(\mathcal{A} \otimes \mathcal{I}_S)\,\rho$.

Remark F.7. Condition (F.5) is only *necessary*, but in general *not sufficient* to guarantee that (F.4) represents a valid physical state. Indeed, the theory may have additional restrictions on the allowed states, as it happens in the presence of superselection rules [80–84]. If the theory is completely unrestricted, such as quantum theory or the theory of quantum supermaps, condition (F.5) and those we derive in the following will be sufficient as well.

Let us analyse the two inequalities in (F.5) separately. If $(\mathcal{A} \otimes \mathcal{I}_S)\,\rho$ is in the cone of states of BS, then we immediately have

$$\left(\rho \begin{array}{c} A \\ S \end{array}\boxed{\mathcal{A}}\begin{array}{c} B \end{array} E\right) \geq 0,$$

for every effect $E \in \mathsf{Eff}\,(BS)$.

Definition F.8. We say that a transformation $\mathcal{A}$ in $\mathsf{Transf}_\mathbb{R}(A, B)$ is *completely positive* if, for every system S and every element $\xi \in \mathsf{St}_+(AS)$, we have $(\mathcal{A} \otimes \mathcal{I}_S)\xi \in \mathsf{St}_+(BS)$.

In words, a completely positive transformation is a linear transformation that maps elements in the input cone of states to elements in the output cone of states in a complete sense, i.e. even when there is an ancillary system S. This is clearly a necessary condition for a transformation to be physical.

Note that it is equivalent to define complete positivity just on states in $\mathsf{St}(AS)$, instead of on generic elements of $\xi \in \mathsf{St}_+(AS)$: $\mathcal{A}$ is completely positive if and only if, for every system S and every state $\rho \in \mathsf{St}(AS)$, we have $(\mathcal{A} \otimes \mathcal{I}_S)\rho \in \mathsf{St}_+(BS)$. To see the non-trivial implication, recall that if ξ is a generic element of $\mathsf{St}_+(AS)$, it can be written as a conical combination of states ρ_i of AS: $\xi = \sum_i \lambda_i \rho_i$, with $\lambda_i \geq 0$ for every i. Then, if we know that $(\mathcal{A} \otimes \mathcal{I}_S)\rho \in \mathsf{St}_+(BS)$ for every $\rho \in \mathsf{St}(AS)$, we have

$$(\mathcal{A} \otimes \mathcal{I}_S)\xi = \sum_i \lambda_i (\mathcal{A} \otimes \mathcal{I}_S)\rho_i \in \mathsf{St}_+(BS),$$

because $\mathsf{St}_+(BS)$ is closed under conical combinations.

Example F.9. In quantum theory, the cone of states is the cone of positive semi-definite operators; therefore completely positive transformations in the sense of definition F.8 are exactly CP maps.

In the theory of quantum supermaps, the cone of states is the cone of CP maps. In this case, completely positive transformations are CPP supermaps [14, 38].

Now let us analyse the second inequality in (F.5), namely

$$\left(\rho \begin{array}{c} \overset{A}{\boxed{\mathcal{A}}} \overset{B}{} \\ S \end{array} E\right) \leq 1, \tag{F.6}$$

for every effect $E \in \mathsf{Eff}(BS)$. Assume $\mathcal{A}$ is completely positive. Then, demanding the validity of inequality (F.6) for every state $\rho \in \mathsf{St}(AS)$ and every effect $E \in \mathsf{Eff}(BS)$ is equivalent to demanding its validity when ρ is any *deterministic* state and E any *deterministic* effect. To see the non-trivial implication, recall that if ρ is non-deterministic, it arises in a preparation-test $\{\rho, \rho'\}$. Similarly, if E is non-deterministic, it arises in an observation-test $\{E, E'\}$. Clearly $\widetilde{\rho} = \rho + \rho'$ is a deterministic state, and $\widetilde{E} = E + E'$ is a deterministic effect. Then

$$1 \geq \left(\widetilde{\rho} \begin{array}{c} \overset{A}{\boxed{\mathcal{A}}} \overset{B}{} \\ S \end{array} \widetilde{E}\right)$$

$$= \left(\rho \begin{array}{c} \overset{A}{\boxed{\mathcal{A}}} \overset{B}{} \\ S \end{array} E\right) + \left(\rho \begin{array}{c} \overset{A}{\boxed{\mathcal{A}}} \overset{B}{} \\ S \end{array} E'\right)$$

$$+ \left(\rho' \begin{array}{c} \overset{A}{\boxed{\mathcal{A}}} \overset{B}{} \\ S \end{array} E\right) + \left(\rho' \begin{array}{c} \overset{A}{\boxed{\mathcal{A}}} \overset{B}{} \\ S \end{array} E'\right).$$

Now, each term in the right-hand side is non-negative because $\mathcal{A}$ is completely positive. It follows that each term is also less than or equal to 1, and specifically

$$\left(\rho \begin{array}{c} \overset{A}{\boxed{\mathcal{A}}} \overset{B}{} \\ S \end{array} E\right) \leq 1.$$

We summarize these necessary requirements in the following theorem.

Theorem F.10. *Let* $\mathcal{A} \in \mathsf{Transf}_\mathbb{R}(A, B)$. *Then* $\mathcal{A}$ *is a physical transformation only if both these conditions are satisfied:*

1. $(\mathcal{A} \otimes \mathcal{I}_S)\rho \in \mathsf{St}_+(BS)$ *for every system* S *and every state* $\rho \in \mathsf{St}(AS)$;

2.

$$\left(\rho \begin{array}{c} \overset{A}{\boxed{\mathcal{A}}} \overset{B}{} \\ S \end{array} u\right) \leq 1,$$

for every system S*, every* deterministic *state* $\rho \in \mathsf{St}(AS)$*, and every* deterministic *effect* $u \in \mathsf{Eff}(BS)$.

Note that in particular, condition 2 implies that

$$\boxed{\rho}\!\!-\!\!\stackrel{A}{-}\!\!\boxed{\mathcal{A}}\!\!\stackrel{B}{-}\!\!\boxed{u} \ \leq 1, \tag{F.7}$$

for it is enough to take S to be the trivial system I. However, in general, this latter condition is *weaker* than condition 2, such as in the theory of quantum supermaps. Let us analyse the role of conditions 1, 2, and (F.7) in this theory.

Example F.11. First of all, since the theory of quantum supermaps has no restrictions, the conditions in theorem F.10 become *sufficient* as well. We have already examined condition 1. Let us focus on condition 2, and unfold its meaning. In this case, ρ is actually a bipartite channel $\mathcal{N}$, and $\mathcal{A}$ acts as a supermap Θ on half of $\mathcal{N}$. Recalling Eq. (F.3), condition 2 becomes $\mathrm{Tr}_{B_1 S_1}\left[\left(\Theta^{A\to B}\otimes \mathbf{1}^S\right)\left[\mathcal{N}^{AS}\right]\left(\rho^{B_0 S_0}\right)\right] \leq 1$. This is nothing but requiring that Θ be completely CPTNI-preserving (cf. Eq. (3.1) in the main article).

In conclusion, the two conditions of theorem F.10 are exactly the two conditions we found in this article. Note that condition (F.7), expressing CPTNI preservation (but not in a complete sense), is *weaker* than condition 2, as there is no way to recover condition 2 from condition (F.7). This is essentially because not all bipartite deterministic effects can be reduced to single-system deterministic effects (cf. Eq. (F.3)). Thus condition (F.7) *cannot* be used to assess whether a candidate supermap is physical or not, so CPTNI preservation is not enough.

If theorem F.10 is valid in all physical theories, why do we not need to impose the trace non-increasing condition in a complete sense in quantum theory? This is because the theory is causal. Indeed in all causal theories, condition 2 becomes equivalent to condition (F.7).

Proposition F.12. *In a causal theory with deterministic effect u, one has*

$$\left(\rho\ \begin{array}{c} \stackrel{A}{\rule{0pt}{0pt}}\boxed{\mathcal{A}}\stackrel{B}{\rule{0pt}{0pt}} \\ \stackrel{S}{\rule{0pt}{0pt}} \end{array}\ \boxed{u}\right) \leq 1,$$

for every system S and every deterministic state $\rho \in \mathsf{St}\,(AS)$, if and only if

$$\boxed{\rho}\!\!-\!\!\stackrel{A}{-}\!\!\boxed{\mathcal{A}}\!\!\stackrel{B}{-}\!\!\boxed{u} \ \leq 1.$$

for every deterministic state $\rho \in \mathsf{St}\,(A)$.

Proof. We have already seen one implication (necessity), now let us focus on the other. Assume condition (F.7) holds. Take an arbitrary system S and an arbitrary deterministic state $\Sigma \in \mathsf{St}\,(AS)$. Then

$$\left(\Sigma\ \begin{array}{c} \stackrel{A}{}\boxed{\mathcal{A}}\stackrel{B}{} \\ \stackrel{S}{} \end{array}\ \boxed{u}\right) = \left(\Sigma\ \begin{array}{c} \stackrel{A}{}\boxed{\mathcal{A}}\stackrel{B}{}\boxed{u} \\ \stackrel{S}{}\boxed{u} \end{array}\right) = \left(\boxed{\rho}\!\!-\!\!\stackrel{A}{-}\!\!\boxed{\mathcal{A}}\!\!\stackrel{B}{-}\!\!\boxed{u}\right) \leq 1,$$

where we have used the fact that the deterministic effect of a composite system factorizes, and that

$$\left(\Sigma\ \begin{array}{c} \stackrel{A}{} \\ \stackrel{S}{}\boxed{u} \end{array}\right) =: \boxed{\rho}\!\!-\!\!\stackrel{A}{-}$$

is a deterministic state. $\qquad\square$

In other words, for causal theories condition 2 can be formulated only for single systems, without the need of an ancillary system S. Recall that in quantum theory u is the trace, so condition (F.7) means that $\mathcal{A}$ is trace-non-increasing. Proposition F.12 is the ultimate reason why in quantum theory it is enough to require that a CP map be TNI (on single system) rather than *completely* TNI. In conclusion, the ultimate origin of the unexpected behaviour of the theory of quantum supermaps is the failure of causality.

However, in [38] one of the authors showed that for a CPP map to be a superchannel, instead, it is not necessary to demand that it be completely TPP, but it is enough that it be TPP. Why do we not need CPTP preservation in a complete sense for superchannels? Let us understand it using the OPT formalism.

Clearly, a superchannel $\Theta^{A\to B}$ must send channels to channels in a complete sense: for any bipartite quantum channel $\mathcal{N}^{AB}$, $\mathbf{1}^R \otimes \Theta^{A\to B}\left[\mathcal{N}^{RA}\right] = \mathcal{M}^{RB}$, where $\mathcal{M}^{RB}$ is still a quantum channel. By Eq. (F.2), this is true if and only if

$$(\mathrm{Tr}_{R_1} \otimes \mathrm{Tr}_{B_1}) \circ \left(\mathbf{1}^R \otimes \Theta^{A\to B}\left[\mathcal{N}^{RA}\right]\right) = \mathrm{Tr}_{R_0} \otimes \mathrm{Tr}_{B_0}, \tag{F.8}$$

where we have denoted the deterministic effect u explicitly as the trace. Now let us try to prove Eq. (F.8) knowing that $\Theta^{A\to B}$ is *just* TPP. Now consider the following channel:

$$\begin{array}{c} \underset{A_0}{\boxed{\mathcal{N}'}}\underset{A_1}{} \quad := \quad \boxed{\rho_0}\!-\!\!\overset{R_0}{\underset{A_0}{\boxed{\mathcal{N}}}}\!\!\overset{R_1}{\underset{A_1}{}}\!\!\boxed{\mathrm{Tr}} \end{array}, \tag{F.9}$$

where ρ_0 is some density matrix on R_0. Since $\Theta^{A\to B}$ is TPP, we have that $\mathcal{M}'^B := \Theta^{A\to B}\left[\mathcal{N}'^A\right]$ is still a quantum channel. In other words

$$\mathrm{Tr}_{B_1} \circ \Theta^{A\to B}\left[\mathcal{N}'^A\right] = \mathrm{Tr}_{B_0}.$$

Then, if we take a density matrix $\sigma_0 \in \mathfrak{D}\left(\mathcal{H}^{B_0}\right)$, we have

$$\mathrm{Tr}_{B_1} \circ \Theta^{A\to B}\left[\mathcal{N}'^A\right]\left(\sigma_0^{B_0}\right) = \mathrm{Tr}_{B_0}\left[\sigma_0^{B_0}\right] = 1.$$

Now, recalling the definition of $\mathcal{N}'^A$ in Eq. (F.9), we have

$$\mathrm{Tr}_{R_1}\mathrm{Tr}_{B_1}\left(\mathbf{1}^R \otimes \Theta^{A\to B}\left[\mathcal{N}^{RA}\right]\right)\left(\rho_0^{R_0} \otimes \sigma_0^{B_0}\right) = 1, \tag{F.10}$$

for any $\rho_0 \in \mathfrak{D}\left(\mathcal{H}^{R_0}\right)$ and any $\sigma_0 \in \mathfrak{D}\left(\mathcal{H}^{B_0}\right)$. If we manage to prove that

$$\mathrm{Tr}_{R_1}\mathrm{Tr}_{B_1}\left(\mathbf{1}^R \otimes \Theta^{A\to B}\left[\mathcal{N}^{RA}\right]\right)\left(\tau^{R_0 B_0}\right) = 1$$

for every bipartite state $\tau^{R_0 B_0}$, then the validity of Eq. (F.8) is shown. Now, recall that in quantum theory every bipartite state can be written as an affine combination of product states. Therefore $\tau^{R_0 B_0} = \sum_j \lambda_j \rho_j^{R_0} \otimes \sigma_j^{B_0}$, with $\sum_j \lambda_j = 1$. Therefore

$$\begin{aligned}\mathrm{Tr}_{R_1}\mathrm{Tr}_{B_1}\left(\mathbf{1}^R \otimes \Theta^{A\to B}\left[\mathcal{N}^{RA}\right]\right)\left(\tau^{R_0 B_0}\right) &= \mathrm{Tr}_{R_1}\mathrm{Tr}_{B_1}\left(\mathbf{1}^R \otimes \Theta^{A\to B}\left[\mathcal{N}^{RA}\right]\right)\left(\sum_j \lambda_j \rho_j^{R_0} \otimes \sigma_j^{B_0}\right) \\ &= \sum_j \lambda_j \mathrm{Tr}_{R_1}\mathrm{Tr}_{B_1}\left(\mathbf{1}^R \otimes \Theta^{A\to B}\left[\mathcal{N}^{RA}\right]\right)\left(\rho_j^{R_0} \otimes \sigma_j^{B_0}\right) \\ &= \sum_j \lambda_j \\ &= 1,\end{aligned}$$

where we have used Eq. (F.10). This proves Eq. (F.8), so for quantum superchannels it is indeed enough to require that they be TPP. Note that this proof does not use any quantum feature except causality, which allows us to characterize quantum channels as CPTP maps, and local tomography [58, 72], a property that guarantees that every deterministic bipartite state can be written as an affine combination of deterministic product states.

The same proof also shows that any attempt to adapt it to supermaps transforming quantum channels to CPTNI maps is bound to fail: even if $\mathrm{Tr}_{R_1}\mathrm{Tr}_{B_1}\left(\mathbf{1}^R \otimes \Theta^{A\to B}\left[\mathcal{N}^{RA}\right]\right)\left(\rho_0^{R_0} \otimes \sigma_0^{B_0}\right) \leq 1$, we cannot conclude that $\mathrm{Tr}_{R_1}\mathrm{Tr}_{B_1}\left(\mathbf{1}^R \otimes \Theta^{A\to B}\left[\mathcal{N}^{RA}\right]\right)\left(\tau^{R_0 B_0}\right) \leq 1$ for every bipartite state $\tau^{R_0 B_0}$. The reason is that we are only dealing with an *affine* combination, possibly even containing negative terms. This does not allow us to conclude anything about $\sum_j \lambda_j \mathrm{Tr}_{R_1}\mathrm{Tr}_{B_1}\left(\mathbf{1}^R \otimes \Theta^{A\to B}\left[\mathcal{N}^{RA}\right]\right)\left(\rho_j^{R_0} \otimes \sigma_j^{B_0}\right)$.

We conclude this Appendix with an interesting remark: sometimes, even with a non-causal theory, the weaker condition (F.7) is enough to characterize which completely positive transformations are physical, in that it becomes equivalent to the stronger condition 2 in theorem F.10. This happens when the only deterministic states of the theory are *separable* [58, 85]: i.e. they can be written as a *convex* combination of product deterministic states. In this case, suppose we know that condition (F.7) holds. Let us assess $(u|\mathcal{A} \otimes \mathcal{I}_S|\Sigma)$, where S is an arbitrary system, $\Sigma \in \mathsf{St}\,(AS)$ is an arbitrary deterministic state, and $u \in \mathsf{Eff}\,(BS)$ is an arbitrary deterministic effect. We have

$$\left(\boxed{\Sigma}\!\!\begin{array}{c}\overset{A}{\boxed{\mathcal{A}}}\overset{B}{}\\\underset{S}{}\end{array}\!\!\boxed{u}\right) = \sum_j p_j \left(\boxed{\alpha_j}\!\!\overset{A}{\boxed{\mathcal{A}}}\overset{B}{}\!\!\boxed{\sigma_j}\!\!\underset{S}{}\,\boxed{u}\right) =: \sum_j p_j \left(\boxed{\alpha_j}\!\!-\!\!\overset{A}{}\boxed{\mathcal{A}}\overset{B}{}\!\!-\!\!\boxed{u_j}\right),$$

where $\{p_j\}$ is a probability distribution, α_j and σ_j are deterministic states, and u_j is the deterministic effect defined as $u_j := u_{\mathrm{BS}} (\mathcal{I}_{\mathrm{B}} \otimes \sigma_{j,\mathrm{S}})$. Now, each term $(u_j | \mathcal{A} | \rho_j) \leq 1$ by condition (F.7), so any convex combination of them will yield a number less than or equal to 1. In this case we were able to prove that condition (F.7) implies condition 2 of theorem F.10.

We can follow the same argument when, dually, all deterministic effects are separable. This is the case of classical supermaps, where the non-product states in the realization of bipartite deterministic effects (Eq. (F.3)) are all separable. Again, let us assume condition (F.7) holds, and let us assess $(u | \mathcal{A} \otimes \mathcal{I}_{\mathrm{S}} | \Sigma)$, where S is an arbitrary system, $\Sigma \in \mathsf{St}\,(\mathrm{AS})$ is an arbitrary deterministic state, and $u \in \mathsf{Eff}\,(\mathrm{BS})$ is an arbitrary deterministic effect, as above. One has

$$
\left(\Sigma \begin{array}{c} \text{A} \boxed{\mathcal{A}} \text{B} \\ \text{S} \end{array} u \right) = \sum_j p_j \left(\Sigma \begin{array}{c} \text{A} \boxed{\mathcal{A}} \text{B} \boxed{u_{j,\mathrm{B}}} \\ \text{S} \boxed{u_{j,\mathrm{S}}} \end{array} \right) =: \sum_j p_j \; \boxed{\sigma_j} \text{—A—} \boxed{\mathcal{A}} \text{—B—} \boxed{u_{j,\mathrm{B}}} \; \leq 1,
$$

where $\{p_j\}$ is a probability distribution, $u_{j,\mathrm{B}}$ and $u_{j,\mathrm{S}}$ are deterministic effects, and σ_j is a deterministic state, defined as $\sigma_j := (\mathcal{I}_{\mathrm{A}} \otimes u_{j,\mathrm{S}})\,\Sigma$. The inequality follows again from condition (F.7).