Cyclic Quantum Causal Models

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We present an extension of the framework of quantum causal models to cyclic causal structures. This offers a novel causal perspective on processes beyond those corresponding to standard circuits, such as processes with dynamical causal order and causally nonseparable processes, including processes that violate causal inequalities. We illustrate the concept with examples of well known causally nonseparable processes. We show that for any directed graph, if a process arises from a unitary process with corresponding causal structure by marginalizing over latent local disturbances, then the process is Markov for that graph. As an application of the approach, we present more fine-grained compositional structures of processes such as the quantum SWITCH, which make the paths of causal influence and information flow graphically evident. Employing this compositional structure, we show that all unitarily extendible bipartite processes are causally separable, with their unitary extensions realizable via coherent control of the order of operations. Finally, we show that for unitary processes, causal nonseparability is equivalent to the cyclicity of their causal structure.

I. INTRODUCTION

There has been growing interest in higher-order quantum processes in which separate operations do not occur in a definite causal order (see, e.g., Refs. \textsuperscript{[1–23]} for a selection). This property, called ‘causal nonseparability’ \textsuperscript{[3–7, 24]}, was formalized within the process matrix framework \textsuperscript{[3]}, which describes correlations between quantum nodes of intervention without assuming a predefined order between the nodes. Challenging conventional notions of causality, causally nonseparable processes have been shown to allow informational tasks that cannot be achieved with operations used in a definite order \textsuperscript{[4–8, 25, 26]}. Such processes have been conjectured to be relevant in the context of quantum gravity \textsuperscript{[1–3, 27]} and closed time-like curves \textsuperscript{[2, 3, 12, 23, 25, 29]}, but some are also known to admit realizations in standard quantum mechanics on time-delocated systems \textsuperscript{[10]}. A prominent example is the quantum SWITCH, which has been demonstrated experimentally \textsuperscript{[30–34]}.

On a separate front, there is the recent development of the framework of quantum causal models \textsuperscript{[35–36]} (see, e.g., Refs. \textsuperscript{[37–48]} for related, previous work) as a fully quantum version of the classical framework of causal models \textsuperscript{[19–50]}. It is formulated within the formalism of process matrices, but contains the classical causal models as special cases and generalizes many of the fundamental concepts and core theorems of the latter. Quantum causal models thus constitute a general framework for reasoning about quantum systems in causal terms, allowing the rigorous study of the empirical constraints imposed by quantum causal structures – however, only as far as causal structures are concerned that are expressible as directed acyclic graphs (DAGs), i.e., where there is a well-defined causal order. The central idea behind the approach in Refs. \textsuperscript{[35–36]} is that causal relations between quantum systems correspond to influence through underlying unitary transformations. This facilitates, in particular, a justification of the quantum Markov condition relative to a DAG that underpins the definition of a quantum causal model – any such model can be thought of as arising from a unitary circuit fragment with a compatible causal structure by marginalizing over latent local disturbances \textsuperscript{[36]}.

In this paper, we merge these hitherto separate lines of research by extending the framework of quantum causal models to processes that are not compatible with a fixed order of the quantum nodes. While this direction of thought has been considered in earlier work (see, e.g., Refs. \textsuperscript{[17–21, 22]}), it was previously not clear how to take the idea forward due to various conceptual and technical obstacles – including, for example, how quantum nodes and the quantum Markov condition should be defined, how the notion of autonomy of causal mechanisms should be understood \textsuperscript{[51]}, and how to prevent paradoxes.

These obstacles are overcome by generalizing the quantum causal models of Refs. \textsuperscript{[35–36]}. For processes that are not compatible with a fixed order of the nodes, the causal structure of the process will now include directed cycles. This may appear counterintuitive, but the process matrix framework guarantees that it is free of paradoxes. What was previously cast simply as indefinite causal order can fruitfully be studied from a causal model perspective in terms of definite, but cyclic, causal structure.

Based on this insight, we define in Sec. \textsuperscript{[III]} the generalized notion of a quantum causal model by dropping the requirement of acyclicity in the definition from Refs. \textsuperscript{[35–36]}. The idea is that quantum causal relations are ultimately to be understood in terms of unitary processes. Sec. \textsuperscript{[IV]} shows that any unitary process has a causal structure that can be represented by a directed graph, and that the unitary process together with its causal structure defines a quantum causal model. This is illustrated in Sec. \textsuperscript{[V]} where it is shown that the quantum SWITCH – a well-known example of a causally nonseparable process – can be understood as a quantum causal model with cyclic causal structure. Sec. \textsuperscript{[VI]} considers the general case of processes not assumed to be unitary, and shows that if a process is compatible with
a given directed graph, i.e., if it can be obtained from a unitary process with a corresponding causal structure by marginalizing over latent local disturbances, then it is Markov for that graph. Proving the converse, however, appears more difficult than in the acyclic case, so we pose it as a conjecture. Sec. VII gives another example, the deterministic classical process found by Araújo and Feix and first presented in Ref. [53], which violates causal inequalities, and shows how it can be understood as a quantum causal model with cyclic causal structure.

The following sections present applications of the approach. By using ‘extended circuit diagrams’, recently introduced in Ref. [54], Sec. VIII presents more fine-grained compositional structures of the quantum SWITCH and the process from Ref. [53], which allow one to understand their causal structures and the flow of information through them. Sec. IX uses this compositional structure to solve the open problem of characterizing all bipartite processes that admit a unitary extension: we show that all such processes are causally separable, with their extensions being variations of the quantum SWITCH. Sec. X uses this compositional structure to solve the open problem of characterizing all multipartite processes, cyclicality of the causal structure and causal nonseparability are equivalent. Finally, Sec. XI formulates the cyclic generalization of classical split-node causal models [56], and provides the classical analogues of various of the quantum results. Sec. XII concludes.

II. BACKGROUND

The process formalism

The process formalism [3] describes the correlations between separate quantum nodes $A_i$, $i = 1, \ldots, n$, each defined by a pair of input and output Hilbert spaces, $\mathcal{H}_{A_{in}}$ and $\mathcal{H}_{A_{out}}$ (here assumed finite-dimensional). At a given quantum node $A$, an agent can apply an arbitrary quantum operation, modeled by a quantum instrument, that is, a collection of completely positive (CP) maps $\{\mathcal{E}^{A}_{k_A} : \mathcal{L}(\mathcal{H}_{A_{in}}) \rightarrow \mathcal{L}(\mathcal{H}_{A_{out}})\}$ corresponding to different possible outcomes $k_A$, where $\mathcal{L}(\mathcal{H})$ is the space of linear operators over $\mathcal{H}$, and such that $\mathcal{E}_A = \sum_{k_A} \mathcal{E}^{k_A}$ is a trace-preserving CP (CPTP) map. Following Refs. [35, 50], we will represent CP maps via positive-semidefinite operators using a basis-independent version of the Choi-Jamiolkowski (CJ) isomorphism [35, 56], which to a given CP map $\mathcal{E} : \mathcal{L}(\mathcal{H}_{A}) \rightarrow \mathcal{L}(\mathcal{H}_B)$ associates the CJ operator $\rho_B^{\mathcal{E}}_{|_{\mathcal{A}}} := \sum_{i,j} \mathcal{E}(|i_A\rangle \langle j|) \otimes |i_A\rangle \langle j|$, where $\{|i_A\rangle\rangle$ is an orthonormal basis of $\mathcal{H}_A$, and $\{|i_A\rangle\rangle$ the corresponding dual basis. For a CPTP map $\mathcal{E}$ it holds $Tr_B[\rho_B^{\mathcal{E}}_{|_{\mathcal{A}}}] = \mathbb{I}_{\mathcal{A}}$. Given a set of instruments at the quantum nodes $A_1, \ldots, A_n$, the joint probability for their outcomes is then given by

$$P(k_{A_1}, \ldots, k_{A_n}) = \text{Tr} \left[ \sigma_{A_1} \cdots A_n \left( \bigotimes_{i=1}^{n} \tau_{A_i}^{k_{A_i}} \right) \right], \quad (1)$$

where $\tau_{A}^{k_{A}} := (\rho_{A_{out|A_{in}}}^{k_{A}})^T$, and $\sigma_{A_1} \cdots A_n \in \mathcal{L}(\otimes_{i} \mathcal{H}_{A_i}^{in} \otimes \mathcal{H}_{A_i}^{out})$ is called the process operator $^{1}$

The only constraints on the latter are [3]: $\sigma_{A_1} \cdots A_n \geq 0$ (required by the non-negativity of probabilities, assuming that the parties can share entangled input ancillas), and $\text{Tr}[\sigma_{A_1} \cdots A_n \left( \tau_{A_1} \otimes \cdots \otimes \tau_{A_n} \right)] = 1$, for any set of CPTP maps $\{\tau_{A_i}\}$ at the $n$ nodes. Simple-to-check necessary and sufficient conditions for an operator in $\mathcal{L}(\otimes_{i} \mathcal{H}_{A_i}^{in} \otimes \mathcal{H}_{A_i}^{out})$ to be a valid process operator can be found in Refs. [40, 41]. To avoid clutter when ‘tracing over’ a node $A$ we will write $\text{Tr}_A[\_] := \text{Tr}_{A_{in}}(A_{out})$, $\_$. $^{1}$

Causal (non)separability

A bipartite process $\sigma_{AB}$ is called causally separable, a property first introduced in Ref. [3], if it can be seen to arise as a convex mixture of processes with a fixed causal order between $A$ and $B$, i.e., if $\sigma_{AB} = p \sigma_{AB}^A + (1-p) \sigma_{AB}^B$, with $0 \leq p \leq 1$ and for some process operator $\sigma_{AB}^A$, which acts trivially on $(A_{out})^*$, so that $A$ cannot signal to $B$, and similarly, $\sigma_{AB}^B$, which acts trivially on $(B_{out})^*$ so that $B$ cannot signal to $A$ [3]. Otherwise $\sigma_{AB}$ is causally nonseparable. In the multipartite case with more than two nodes, there are more intricate notions of causal separability, beyond just convex mixtures of fixed causal orders, in particular notions which allow for a dynamical causal order and ‘activation of causal nonseparability’ through shared entangled auxiliary input systems for all nodes. A formal definition is given in Sec. X. See also Refs. [7, 24] for a detailed discussion.

III. QUANTUM CAUSAL MODELS

The following definition generalizes that of Refs. [35, 36], by allowing cyclic graphs, and by allowing that the input and output Hilbert spaces of a quantum node can have different dimensions.

Definition 1. (Quantum causal model (QCM) — generalized): A QCM is given by:

1. a causal structure represented by a directed graph $G$ with vertices corresponding to quantum nodes $A_1, \ldots, A_n$,
2. for each $A_i$, a quantum channel $\rho_{A_i|Pa(A_i)} \in \mathcal{L}(\mathcal{H}_{A_{in}}^{in} \otimes \mathcal{H}_{Pa(A_i)_{out}}^{out})$, where $Pa(A_i)$ denotes the set of parents of $A_i$ according to $G$, such that
[\rho_{A_i|Pa(A_i)} , \rho_{A_j|Pa(A_j)}] = 0 \text{ for all } i, j \text{ and such that } \sigma_{A_1...A_n} = \prod_i \rho_{A_i|Pa(A_i)} \text{ is a process operator over the quantum nodes } A_1, ..., A_n.

When writing products of the form \( \prod_i \rho_{A_i|Pa(A_i)} \), it is understood implicitly that each factor is ‘padded’ with an identity operator in tensor product for all other spaces. A QCM is called cyclic iff its causal structure contains directed cycles, and acyclic otherwise.

![Figure 1: Examples of cyclic directed graphs.](image)

Not every cyclic graph supports a QCM in an interesting way. Consider, for example, the two-node cyclic graph of Fig. 1a. Such a causal structure would come with a process operator

\[
\sigma_{AB} = \rho_{A|B} \rho_{B|A}
\]

(2)

Here and throughout, channels between the nodes on which a process is defined are written such that anything appearing to the right of the bar refers to the output Hilbert space of the node, and anything appearing to the left of the bar refers to the input Hilbert space of the node. By our conventions \( \rho_{A|B} \rho_{B|A} = \rho_{A|B} \otimes \rho_{B|A} \). However, this is not a valid process operator unless either \( \rho_{A|B} = \rho_{A\text{in}} \otimes \mathbf{1}_{B\text{out}} \), or \( \rho_{B|A} = \rho_{B\text{in}} \otimes \mathbf{1}_{A\text{out}} \). In other words, for \( \sigma_{AB} \) to be a valid process operator, it must be the case that at least one of the channels \( \rho_{A|B} \) and \( \rho_{B|A} \) does not permit signals to be sent from the input of the channel to the output of the channel. Intuitively speaking, this is because such a situation would lead to logical paradoxes for certain choices of interventions at \( A \) and \( B \).

More generally, let us say that a channel \( \rho_{CD|AB} \) is non-signalling from input system \( A \) to output system \( D \) iff \( \rho_{D|AB} = \text{Tr}_C[\rho_{CD|AB}] = \rho_{D|B} \otimes \mathbf{1}_A \). Let us also say that a QCM is faithful iff each of the channels \( \rho_{A_i|Pa(A_i)} \) is signalling from \( A_i \text{out} \) to \( A_i \text{in} \) for every \( A_i \in Pa(A_i) \). Our claim concerning the causal structure of Fig. 1a can be summarized as:

**Proposition 1.** There is no faithful cyclic quantum causal model with two nodes.

For a proof, see App. B

Now consider the cyclic graph \( G' \) in Fig. 1b. A QCM with \( G' \) as its causal structure comes with the data

\[
\sigma_{ABC} = \rho_{A|BC} \rho_{B|AC} \rho_{C}
\]

(3)

Eq. 3 compared to Eq. 2 has the key difference that the commuting operators have non-trivial action on \( (\text{Out})^* \). As a result, it turns out that faithful cyclic QCMs of this form do exist. An example is described below in Sec. X.

Note that, given a cyclic graph such as that in Fig. 1b, even when a faithful QCM exists it is not in general the case that any set of commuting channels \( \rho_{A_i|Pa(A_i)} \) defines a process operator. (See App. C for an explicit demonstration of this fact.) The constraint in the definition of a QCM that \( \sigma_{A_1...A_n} = \prod_i \rho_{A_i|Pa(A_i)} \) is a valid process operator is essential, and is what guarantees that grandfather-type paradoxes do not arise \(^3\). This is in contrast to the acyclic case, where, given an acyclic causal structure, it is not hard to argue that any product of commuting channels of the form \( \prod_i \rho_{A_i|Pa(A_i)} \) is a valid process operator \(^3\), hence in particular a faithful QCM with that causal structure can always be found.

For future reference, it is useful to define a term to express the fact that a given process operator \( \sigma \) has the correct form with respect to a given causal structure to define a QCM.

**Definition 2.** (Quantum Markov condition — generalized): A process \( \sigma_{A_1...A_n} \) is called Markov for a directed graph \( G \) with quantum nodes \( A_1, ..., A_n \) as its vertices iff it admits a factorization into pairwise commuting channels of the form \( \sigma_{A_1...A_n} = \prod_i \rho_{A_i|Pa(A_i)} \).

**IV. UNITARITY AND CAUSAL STRUCTURE**

The definition of a QCM above is predicated on the idea that causal structure should be represented by a directed graph. This idea, however, along with the stipulation that the accompanying process is Markov for the graph, was presented without much justification or further comment. Why is causal structure represented by a directed graph, for example, as opposed to a different mathematical object, such as a partial order, or a preorder, or some kind of hypergraph? This section considers a subclass of processes – unitary processes, defined momentarily – and shows that a unitary process is associated with a causal structure, which can indeed be represented with a directed graph, and that the unitary process is Markov for that graph. In other words, a unitary process, along with its causal structure, defines a QCM.

In order to define a unitary process, observe that a process operator \( \sigma_{A_1...A_n} \) has the mathematical form of the CJ operator for a channel \( \mathcal{P} : \mathcal{L}(\otimes_i \mathcal{H}_{A_i\text{out}}) \to \mathcal{L}(\otimes_i \mathcal{H}_{A_i\text{in}}) \) where it is convenient to emphasize this form, we will sometimes write \( \sigma_{A_1...A_n} = \rho_{A_1...A_n|A_1...A_n} \), where it is understood implicitly that an ‘\( A_i \)’ to the right of the ‘bar’ stands for \( A_i\text{out} \), while

\(^2\)This follows from the constraint expressed in Eq 1. The constraint is stronger than the mere fact that the process operator defines a channel, hence not any channel \( \mathcal{P} : \mathcal{L}(\otimes_i \mathcal{H}_{A_i\text{out}}) \to \mathcal{L}(\otimes_i \mathcal{H}_{A_i\text{in}}) \) defines a process operator.
an ‘A,’ to the left of the bar stands for A\textsuperscript{in}. A unitary process is a process (where some of the input or output spaces may be trivial, i.e., 1-dimensional) such that the channel \( \mathcal{P} \) is a unitary channel.

The first step is to define a notion of causal structure that pertains to the inputs and outputs of a unitary channel.

**Definition 3.** (Causal structure of a unitary channel): Given a unitary channel \( \rho_{\mathcal{DAB}}^{\mathcal{C}} \), write \( A \rightarrow D \) (‘A does not influence D’), iff \( \text{Tr}_C(\rho_{\mathcal{DAB}}^{\mathcal{C}}) = \rho_{\mathcal{D}B}^{\mathcal{M}} \otimes I_A \) for some marginal channel \( \mathcal{M} \). If A can influence D, i.e., \( \neg(A \rightarrow D) \), A is a direct cause of D. For any unitary channel \( \rho_{\mathcal{CD}B}^{\mathcal{C}} \) with k input and l output subsystems its causal structure is then the set of causal relations between input and output subsystems and can be represented by a DAG with vertices \( B_1, \ldots, B_k \) and \( C_1, \ldots, C_l \) and an arrow \( B_j \rightarrow C_i \) whenever \( B_j \) is a direct cause of \( C_i \).

This definition lifts naturally to the case of a unitary process, in such a way that causal relationships are defined between the nodes of the process, rather than between inputs and outputs of a channel.

**Definition 4.** (Causal structure of a unitary process): Given a unitary process \( \sigma_{A_1 \ldots A_n} = \rho_{A_1 \ldots A_n|A_1 \ldots A_n}^{\mathcal{M}} \), write \( A_j \rightarrow A_i \) (‘node \( A_j \) does not influence node \( A_i \)’), iff \( A_i^{\text{out}} \) does not influence \( A_j^{\text{in}} \) in \( \mathcal{U} \). If node \( A_j \) can influence node \( A_i \), then \( A_i \) is a direct cause of \( A_j \). The causal structure of the unitary process is the set of all causal relations between its quantum nodes, and is representable as the directed graph with vertices \( A_1, \ldots, A_n \) and an arrow \( A_j \rightarrow A_i \), whenever \( A_j \) is a direct cause of \( A_i \).

The fact that any unitary process is Markov for its causal structure, hence defines a QCM, is then immediate from the following theorem of Refs. [35, 36].

**Theorem 1.** [35, 36]: Given a unitary channel \( \rho_{\mathcal{CD}B}^{\mathcal{C}} \), let \( \{P_a(C_i)\}_{i=1} \) be the parental sets as defined by its causal structure. Then the CJ operator factorizes as \( \rho_{\mathcal{CD}B}^{\mathcal{C}} = \prod_{i=1} \rho_{C_i|P_a(C_i)} \cdot \rho_{C_i|P_a(C_i)} = 0 \) for all \( i, j \).

How about non-unitary processes? It will be noticed that according to Def. 3, \( A \rightarrow D \) in the unitary channel \( \rho_{\mathcal{CD}B}^{\mathcal{C}} \) precisely if \( \rho_{\mathcal{CD}B}^{\mathcal{C}} \) is non-signalling from \( A \) to \( D \) according to the definition given in Sec. [1]. There is a reason, though, why Def. 3 is restricted to unitary channels, and why the definition is phrased in terms of causal influence, rather than signalling. In a non-unitary channel \( \rho_{\mathcal{CD}B}^{\mathcal{C}} \), it can happen that \( A \) does not signal to \( C \) and \( A \) does not signal to \( D \), yet \( A \) does signal to the composite system \( CD \). In the unitary case, on the other hand, Thm. 1 ensures that this cannot happen. This means that the signalling structure of a general channel is not fully specified by listing, for each output, which inputs can signal to it. Rather, arbitrary subsets of outputs must be considered, and the signalling structure of a general channel cannot be represented by a graph with arrows from inputs to outputs. Similar remarks apply to a general process \( \sigma_{A_1 \ldots A_n} = \rho_{A_1 \ldots A_n|A_1 \ldots A_n}^{\mathcal{M}} \), thought of as a channel from the output Hilbert spaces of nodes to the input Hilbert spaces. Specification of all the possibilities for signalling in the process requires consideration of arbitrary subsets of nodes, and – unlike in the case of unitary processes – cannot be summarized with a directed graph defined over the nodes.

The case of non-unitary processes, and their relationship to causal structure is presented in Sec. [VI]. First, we describe a well-known example of a causally nonseparable process – the quantum SWITCH [2] – and show explicitly that it defines a unitary process operator with cyclic causal structure, hence a cyclic QCM.

**V. EXAMPLE: THE QUANTUM SWITCH**

The quantum SWITCH [2] was the first example described of a causally non-separable process. The SWITCH is standardly defined as a higher-order map \( F_{\text{SWITCH}} : \mathcal{L}(H_A^{\text{in}}) \rightarrow \mathcal{L}(H_A^{\text{out}}) \) and \( G_B : \mathcal{L}(H_B^{\text{in}}) \rightarrow \mathcal{L}(H_B^{\text{out}}) \), where \( d_{\text{in}} = d_{\text{out}} = d = d_{\text{in}} = d_{\text{out}} = d \), and gives as an output a CP map \( E : \mathcal{L}(H_Q \otimes H_S) \rightarrow \mathcal{L}(H_{Q' \otimes H_{S'}}) \), where \( d_Q = d_{Q'} = 2 \) and \( d_S = d_{S'} = d \). Here, \( H_Q \) and \( H_{Q'} \) are interpreted as the Hilbert spaces of a control qubit at some initial and some final time, respectively, and \( H_S \) and \( H_{S'} \) as the Hilbert spaces of some target system at the same two times. Intuitively, the effect of the quantum SWITCH is to transform the target system from the initial to the final time by the sequential application of the CP maps \( F_A \) and \( G_B \), where the order in which the two CP maps are applied is conditioned coherently on the logical value of the control qubit.

To formulate this precisely, we will describe the quantum SWITCH directly as a 4-node process (see Fig. 2), which involves the nodes \( A \) and \( B \), where \( F_A \) and \( G_B \) are inserted, a node \( P \) with \( P^{\text{out}} = QS \), where the control qubit and target system at the initial time are prepared in some state, and node \( F \) with \( F^{\text{in}} = Q' S' \), where the control qubit and the system at the final time are subject to some measurement. The SWITCH is then a unitary four-partite process with process operator \( \sigma_{A^{\text{SWITCH}}}^{P} = \rho_{A^{\text{SWITCH}}B^{P}}^{QS} = |W\rangle\langle W| \), where

\[
|W\rangle := |0\rangle_Q |0\rangle_Q' |\phi^+\rangle_{S'A^{\text{in}}} |\phi^+\rangle_{(A^{\text{out}})B^{\text{in}}} |\phi^+\rangle_{(B^{\text{out}})S'} + |1\rangle_Q |1\rangle_Q' |\phi^+\rangle_{S'B^{\text{in}}} |\phi^+\rangle_{(B^{\text{out}})S'} ,
\]

with \( |\phi^+\rangle_X := \sum_i |i\rangle_X |i\rangle_Y \) and the appearance of the dual spaces due to our convention for the CJ isomorphism. It is straightforward to verify that the causal structure of \( \sigma_{A^{\text{SWITCH}}}^{P} \) is the cyclic directed graph in Fig. 3. From Thm. 1 it follows that

\[
\sigma_{A^{\text{SWITCH}}}^{P} = \rho_{F^{P}A^{P}B^{P}B^{P}A^{P}P} \rho_{P} \rho_{P} \rho_{P} \rho_{P} \rho_{P} .
\]
where we have formally added $\rho_P$ to make the Markovianity of $\sigma^{\text{SWITCH}}_{\text{ABPF}}$ for $G_{\text{SWITCH}}$ explicit, but here $\rho_P$ is just the number 1, since $P^{\text{in}}$ is trivial. Hence, the graph $G_{\text{SWITCH}}$ together with $\rho_{P|ABP}, \rho_{A|BP}, \rho_{B|AP}, \rho_P, \rho_P$, form a faithful cyclic QCM.

VI. COMPATIBILITY VS MARKOVIANITY

As argued at the end of Sec. IV, the possibilities for signalling in a generic process $\sigma_{A_1...A_n} = \rho_{P|A_1...A_n}^{\text{in}}$ cannot be represented with a directed graph on the nodes. Hence the idea of a quantum causal model is certainly not that one may write down a generic process $\sigma_{A_1...A_n}$ along with a graph that describes the possibilities for signalling. Instead, the graph represents an underlying causal structure that constrains the process, hence constrains any correlations between outcomes of interventions at the nodes.

What is this causal structure, and why does it impose a constraint on the process in the form of the Markov condition? The provisional approach taken in this work, in common with Refs. [35, 36], is that quantum causal relations are always defined by unitary processes. In a QCM involving a non-unitary process $\sigma$, the arrows of the graph are taken to represent facts about the causal structure of some unitary process, with the property that $\sigma$ is recovered from the unitary process when marginalising over auxiliary systems. The unitary process is either known, or is hypothesised as a candidate causal explanation for the correlations inherent in a specified process $\sigma$.

The following was introduced in Ref. [59], and will help make these ideas precise.

**Definition 5.** (Unitary extendibility): A process $\sigma_{A_1...A_n}$ is called unitarily extendible if there exists a unitary process $\sigma_{A_1...A_n}^{P|F} = \rho_{A_1...A_n}^{P|F|A_1...A_n}$ on the quantum nodes $A_1, \ldots, A_n$, plus additional root node $P$ and leaf node $F$, such that $\sigma_{A_1...A_n} = \operatorname{Tr}_F\rho_{A_1...A_n}^{P|F} \rho_P$ for some state $\rho_P \in \mathcal{L}(\mathcal{H}_P)$. The process $\sigma_{A_1...A_n}^{P|F}$ is called a unitary extension of $\sigma_{A_1...A_n}$.

Importantly, it was found in Ref. [59] that not all process operators are unitarily extendible. The reason for this is that, although for any process $\sigma_{A_1...A_n} = \rho_{A_1...A_n}^{P|F|A_1...A_n}$, corresponding to a channel $\mathcal{P}$, the channel $\mathcal{P}$ admits a dilation to a unitary channel, this unitary channel does not necessarily correspond to a valid process itself. Process operators that are not unitarily extendible are those for which no dilation exists such that the unitary channel corresponds to a valid process.

Now suppose that a process $\sigma_{A_1...A_n}$ does have a unitary extension $\sigma_{A_1...A_n}^{P|F}$, involving the additional root node $P$. As per Def. 4, the unitary extension $\sigma_{A_1...A_n}^{P|F}$ has a causal structure given by some directed graph $G$ with nodes $A_1, \ldots, A_n, P, F$. Let $G'$ be the subgraph with nodes $A_1, \ldots, A_n$, along with all arrows that connect only these nodes in $G$. In general, in the graph $G$, the node $P$ will have arrows to several of the $A_i$, meaning that $P$ is a common cause for these nodes. Under the supposition that the unitary extension $\sigma_{A_1...A_n}^{P|F}$ represents the actual state of affairs, there will in general be correlations inherent in $\sigma$ that are explained by the common cause $P$. This means that the graph $G'$, which omits $P$, is at best an incomplete causal explanation for the correlations inherent in $\sigma$, since it does not explain those correlations due to $P$.

We are interested, therefore, in unitary extensions of $\sigma_{A_1...A_n}$ with the feature that the node $P$ can be factored into uncorrelated local disturbances $\lambda_i$, such that each $\lambda_i$ is a cause of only one of the nodes $A_i$. This way, the graph $G'$, obtained by omitting all of the $\lambda_i$ and leaf node $F$, may serve as a candidate causal explanation for correlations described by the process $\sigma_{A_1...A_n}$, which omits only local disturbances and the final effect $F$, and which does not omit common causes. In this case, we will say that $\sigma$ is compatible with the graph $G'$. In fact, it is more useful to define this term more broadly: we will say that $\sigma$ is compatible with any graph, with nodes $A_1, \ldots, A_n$, that contains $G'$ as a subgraph. The following definition makes this precise, generalizing that of Ref. [30] to the cyclic case.
Definition 6. (Compatibility with a directed graph): A process $\sigma_{A_1...A_n}$ is compatible with a directed graph $G$ with nodes $A_1, ..., A_n$, iff $\sigma_{A_1...A_n}$ is extendable to a unitary process $\sigma_{A_1...A_n\lambda_1...\lambda_nF}$, with an extra root node $\lambda_i$ for $i = 1, ..., n$ and an extra leaf node $F$, such that:

1. there exists a product state $\tau_{\lambda_1} \otimes \cdots \otimes \tau_{\lambda_n}$ with $\tau_{\lambda_i} \in \mathcal{L}(\mathcal{H}_{\text{out}_i})$ such that $\sigma_{A_1...A_n} = \text{Tr}_{A_1...A_nF} \{ \sigma_{A_1...A_n\lambda_1...\lambda_nF} (\tau_{\lambda_1} \otimes \cdots \otimes \tau_{\lambda_n}) \}$.

2. $\sigma_{A_1...A_n\lambda_1...\lambda_nF}$ satisfies the following no-influence conditions (with $Pa(A_i)$ referring to $G$): $\{ A_j \rightarrow A_i \}_{A_j \notin Pa(A_i)}$; $\{ \lambda_j \rightarrow A_i \}_{j \neq i}$.

The following then justifies the stipulation, as a part of the definition of a QCM, that the process accompanying a graph is Markov for the graph.

Theorem 2. If a process $\sigma_{A_1...A_n}$ is compatible with the directed graph $G$, then it is also Markov for $G$.

Proof: Similarly to the acyclic case in Ref. [36], the theorem follows essentially from Thm. 1, the unitary extension, asserted to exist by virtue of the theorem follows essentially from Thm. 1: the causal constraints can always be found [36], it is not though a dilation to a unitary channel with the required product of three qubits $P$, which are incompatible with the existence of a dilation to a unitary channel with the required product of three qubits $P$. As is explicit in this description, the AF process together with the causal structure in Fig. 4 defines a faithful cyclic QCM.

It was shown by Baumeler and Wolf (BW) [65] that this process is unitarily extendible (also see Refs. [29, 59]) with a unitary extension given by

$$\sigma^\text{uw}_{ABC,F} = \rho_{ABC,F} \rho_B |CA \rho_C|AB, \quad \text{where}$$

$$\rho_A|BC = \sum_{b,c=0,1} |¬b \land c\rangle \langle ¬b \land c|_{A\text{\text{in}}} \otimes |b,c\rangle_{B\text{\text{out}}C\text{\text{out}}},$$

$$\rho_B|CA = \sum_{c,a=0,1} |¬c \land a\rangle \langle ¬c \land a|_{C\text{\text{in}}} \otimes |c,a\rangle_{C\text{\text{out}}A\text{\text{out}}},$$

$$\rho_C|AB = \sum_{a,b=0,1} |¬a \land b\rangle \langle ¬a \land b|_{B\text{\text{in}}} \otimes |a,b\rangle_{A\text{\text{out}}B\text{\text{out}}}. \quad (6)$$

As is explicit in this description, the AF process together with the causal structure in Fig. 4 defines a faithful cyclic QCM.

The original AF process is recovered for marginalization over $F$ and feeding in the product state $|0,0,0\rangle$ for $\lambda_A$, $\lambda_B$ and $\lambda_C$. Formally letting the latter three define distinct root nodes $\lambda_A$, $\lambda_B$ and $\lambda_C$, it is not too hard to show that this BW unitary extension also satisfies the corresponding causal constraints of Def. 13 to establish $\sigma^\text{uw}_{ABC}$ to be compatible with the graph of Fig. 4 — in keeping with Conjecture 1.

VIII. CYCLICITY AND EXTENDED CIRCUIT DIAGRAMS

An essential feature of the Markov condition in Def. 2 is the pairwise commutation relation of the operators

3See Ref. [15] for the acknowledgement of the discovery of this process by M. Araújo and A. Feix.
of the form \( \rho_{A_i|P_{\alpha(A_i)}} \), where the parental sets in general overlap. That two commuting operators act non-trivially on the same Hilbert space has consequences for the algebraic structure of the operators and leads to an intimate link between causal and compositional structure. The following will exemplify the fruitfulness of studying this link.

Looking inside the quantum SWITCH

As discussed in Sec. VIII the quantum SWITCH can be considered as a unitary process over 4 nodes, given by \( \sigma_{\text{SWITCH}}^{ABPF} = \rho_{ABF}^{A_i} = |W\rangle \langle W| \), where \(|W\rangle\) is defined in Eq. 4. The unitary channel \( \mathcal{U} \) corresponds to a unitary map \( \mathcal{U} : \mathcal{H}_{A_{\text{out}}} \otimes \mathcal{H}_{p_{\text{out}}} \otimes \mathcal{H}_{q_{\text{out}}} \rightarrow \mathcal{H}_{A_{\text{in}}} \otimes \mathcal{H}_{F_{\text{in}}} \otimes \mathcal{H}_{B_{\text{in}}} \), which is depicted in Fig. 5 together with its causal structure shown in blue. Observe in particular that in \( \mathcal{U} \), \( A_{\text{out}} \) does not influence \( A_{\text{in}} \), and similarly \( B_{\text{out}} \) does not influence \( B_{\text{in}} \), as must be the case for a well-defined process [19].

Ref. [53] shows that any unitary map \( \mathcal{U} \) with three in- and output systems, and the causal constraints of Fig. 5 has a decomposition of the following form:

\[
U = \left( \mathbf{1}_{A_{\text{in}}} \otimes T \otimes \mathbf{1}_{A_{\text{in}}} \right) \left( \bigoplus_{i \in I} V_i \otimes W_i \right) \left( \mathbf{1}_{A_{\text{out}}} \otimes S \otimes \mathbf{1}_{B_{\text{out}}} \right), \tag{8}
\]

where \( S \) and \( T \) are unitaries, and \( \{V_i\}_{i \in I} \) and \( \{W_i\}_{i \in I} \) families of unitaries such that

\[
S : \mathcal{H}_{p_{\text{out}}} \rightarrow \bigoplus_{i \in I} \mathcal{H}_{P_{i}^L} \otimes \mathcal{H}_{P_{i}^R},
\]

\[
V_i : \mathcal{H}_{A_{\text{out}}} \otimes \mathcal{H}_{P_{i}^L} \rightarrow \mathcal{H}_{B_{\text{in}}} \otimes \mathcal{H}_{F_{i}^+},
\]

\[
W_i : \mathcal{H}_{P_{i}^R} \otimes \mathcal{H}_{q_{\text{out}}} \rightarrow \mathcal{H}_{F_{i}^+} \otimes \mathcal{H}_{A_{\text{in}}},
\]

Such a compositional structure with direct sums over tensor products goes beyond what is expressible with ordinary circuit diagrams. Ref. [54] therefore introduced extended circuit diagrams to give a graphical representation of such decompositions. Fig. 6 arises from that extended circuit diagram representation of Eq. 8 by bending the wires corresponding to \( A_{\text{in}} \) and \( B_{\text{in}} \) down to re-identify the quantum nodes \( A \) and \( B \) thereby ‘filling the black box’ of the quantum SWITCH from Fig. 2. For details on this diagrammatic language we refer the reader to Ref. [54], but the essential idea is that individual wires with indices on them, such as those between the circles \( S \) and \( V_i \) and \( W_i \), respectively, represent the families of Hilbert spaces \( \{\mathcal{H}_{P_{i}^L}\}_{i \in I} \) and \( \{\mathcal{H}_{P_{i}^R}\}_{i \in I} \), while the two parallel wires together represent \( \bigoplus_{i \in I} \mathcal{H}_{P_{i}^L} \otimes \mathcal{H}_{P_{i}^R} \). An implicit summation over orthogonal subspaces indexed by \( i \) allows the representation of the intermediate unitary map \( \bigoplus_{i \in I} V_i \otimes W_i \) from Eq. 8.

It is easy to see what this decomposition is concretely in the case of the quantum SWITCH: the index \( i \) takes two values, 0 and 1, corresponding to the logical values of the control qubit, i.e., \( \mathcal{H}_P = \mathcal{H}_Q \otimes \mathcal{H}_S \cong (\mathbb{C} \otimes \mathcal{H}_S) \oplus (\mathcal{H}_S \otimes \mathbb{C}) \) and the unitaries \( V_i \) and \( W_i \) are either the SWAP transformation on the respective systems or the identity depending on \( i \). We see that even though the causal structure of the full process is cyclic, the process splits into a direct sum of processes in each of which causal influence and the flow of information follow acyclic paths.

This decomposition of the quantum SWITCH applies more generally: seeing as any unitary process of the type depicted in Fig. 2 with a root node \( P \), a leaf node \( F \), and two nodes \( A \) and \( B \) ‘in between’, satisfies \( A_{\text{out}} \rightarrow A_{\text{in}} \)
and $B^\text{out} \rightarrow B^\text{in}$, it follows that any such unitary process has a decomposition as in Fig. 6. As will be shown in Sec. IX, Thm. 3, all such processes are in fact direct sums of processes in which causal influences flow along acyclic paths.

Looking inside the BW unitary extension of the AF process

Section VII presented the tripartite AF process and its BW unitary extension $\rho^\text{U}_{ABC|A|BC}$ (see Eqs. (6)-(7)). The root node $P$ has as output space $\mathcal{H}_{\text{pout}} = \mathcal{H}_A \otimes \mathcal{H}_{\lambda_B} \otimes \mathcal{H}_{\lambda_C}$, where each $\lambda_X$ influences only $X$ and $F$ for $X = A, B, C$. The associated unitary map $U$ and its causal structure are depicted in Fig. 7. The results from Ref. [54] (essentially Thm. 7 therein) allow again the statement of an extended circuit decomposition of $U$, which is implied by its causal structure and which makes the pathways of causal influence through $U$ graphically evident. This decomposition of $U$ is depicted in Fig. 8 and reads:

$$U = \left( \mathbb{1}_{C^\text{in}B^\text{in}A^\text{in}} \otimes W \right) \left( \bigoplus_{i,j,k} P_{ij} \otimes Q_{ik} \otimes R_{jk} \right) \left( \mathbb{1}_{\lambda_A} \otimes S \otimes \mathbb{1}_{\lambda_B} \otimes T \otimes V \otimes \mathbb{1}_{\lambda_C} \right),$$  \hspace{1cm} (9)

for (families of) unitary maps

$$S : \mathcal{H}_{A^\text{out}} \rightarrow \bigoplus_i \mathcal{H}_{X_i^L} \otimes \mathcal{H}_{X_i^R},$$

$$T : \mathcal{H}_{B^\text{out}} \rightarrow \bigoplus_i \mathcal{H}_{Y_i^L} \otimes \mathcal{H}_{Y_i^R},$$

$$V : \mathcal{H}_{C^\text{out}} \rightarrow \bigoplus_i \mathcal{H}_{Z_i^L} \otimes \mathcal{H}_{Z_i^R},$$

$$W : \bigoplus_{i,j,k} \mathcal{H}_{G_{ij}^{(1)}} \otimes \mathcal{H}_{G_{ik}^{(2)}} \otimes \mathcal{H}_{G_{jk}^{(3)}} \rightarrow \mathcal{H}_{F^\text{in}},$$

$$P_{ij} : \mathcal{H}_{\lambda_C} \otimes \mathcal{H}_{X_i^L} \otimes \mathcal{H}_{Y_j^L} \rightarrow \mathcal{H}_{C^\text{in}} \otimes \mathcal{H}_{G_{ij}^{(1)}},$$

4The proof of the decomposition in Eq. (9) goes through completely analogously to that of Thm. 7 in Ref. [54], since the only difference here is that there are three further input systems $\lambda_A$, $\lambda_B$ and $\lambda_C$ with $\lambda_X$ only influencing $X$ and $F$ for $X = A, B, C$.

5This is a different use of the term ‘faithful’ from that defined earlier according to which a QCM is either ‘faithful’ or not.
of input Hilbert spaces and output Hilbert spaces) have a causally faithful extended circuit decomposition. This would mean that all unitary processes, by bending the wires, would admit causally faithful decompositions in a similar manner. At the time of writing, however, the hypothesis remains unproven.

IX. THE BIPARTITE UNITARILY EXTENDIBLE PROCESSES

Understanding which processes have a physical realization is a central open question in the field of ‘indefinite causal order’ [19]. While causally nonseparable processes may have a realization in exotic scenarios involving both quantum systems and gravity, it seems clear that any present-day laboratory experiment admits a description in terms of a straightforward, definite, causal ordering of suitably defined parts of the experiment. Nevertheless, various experiments have been performed that are claimed as realizations of nonseparable processes such as the quantum SWITCH [30–34, 66]. This raises the question: which processes in general admit a laboratory implementation, at least in terms of time-delocalized systems? In particular, can a process violating causal inequalities be implemented?

There was some hope that a process violating causal inequalities could be implemented, because Ref. [19] also shows that every unitary extension of a bipartite process has a realization in terms of time-delocalized systems. Hence if there were a unitarily extendible bipartite process violating causal inequalities, then it could be implemented, at least via time-delocalized systems. The following theorem, however, shows that there is no such possibility. Any bipartite unitarily extendible process is causally separable, hence in particular cannot violate causal inequalities, as conjectured in Ref. [59]; furthermore, all unitary extensions of bipartite processes are variations of the quantum SWITCH, realizable by coherent control of the times of the operations of A and B. The argument uses the existence of a faithful extended circuit decomposition of the form as in Eq. 8 that is implied by the causal constraints of Fig. 5.

Theorem 3. All unitarily extendible bipartite processes are causally separable. Given a bipartite process, if it is unitarily extendible, then the unitary extension has a realization in terms of coherent control of the order of the node operations.

Proof: See App. D.

As one can see, e.g., from the AF process, being unitarily extendible does not imply causal separability in the general multipartite case. However, suppose a causally faithful extended circuit decomposition of the unitary extension of some multipartite process is known, as is the case for the BW unitary extension of the AF process (see again Sec. VIII). It is then natural to ask whether some kind of generalization of the constraints established as part of the proof of Thm. 3 could be derived, which in the bipartite case just happen to give causal separability. This could also provide insights into the potential implementability of such processes. We leave these questions for future investigation.

X. CAUSAL NONSEPARABILITY

Sec. II gave the definition of causal separability of a process for the bipartite case. As mentioned, in the multipartite case, with more than two nodes, the notion of causal separability is more intricate, allowing for

6It was also shown in Ref. [19] that a specific class of isometric processes has a similar realization in terms of time-delocalized systems. It is presently not known whether that class is unitarily extendible.
the phenomenon of dynamical causal order, in which the causal order of some nodes can depend on earlier nodes. This section gives a precise definition of causal nonseparability. The main result is then that a unitary process is causally nonseparable if and only if it has a cyclic causal structure.

We will use a notion of causal separability that is preserved under extending the process with an arbitrary ancillary input state shared between the nodes. This was originally called extensible causal separability in Ref. [7]. Here we simply refer to it as causal separability, as in Ref. [24] The definition relies on the notion of no-signalling in a process. The following definition of no-signalling, along with various equivalent statements, is given in Ref. [4].

**Definition 7.** (No signalling in a process): Given a process \( \sigma_{A_1...A_n} \), we say that there is no signalling from a subset \( S \subset \{A_1,...,A_n\} \) of its nodes to the complementary subset \( \bar{S} := \{A_1,...,A_n\} \setminus S \), iff the probabilities \( P(k_S) = \text{Tr} \left[ \sigma_{A_1...A_n} \left( \tau^k_S \otimes \tau^k_S \right) \right] \) for the outcomes of any operation \( k_S = \bigotimes_{A \in S} \tau^k_A \) performed at \( \bar{S} \) are independent of the choice of trace-preserving operations \( \tau_S = \bigotimes_{A \in S} \tau_A \) performed at \( S \).

Now let \( \tau_A \) represent a CP map at the node \( A \), which is not necessarily trace-preserving. If there is no signalling to a node \( A \) from \( \{A_1,...,A_n\} \setminus \{A\} \), then for any \( \tau_A \), the object \( \text{Tr}_A [\sigma_{A_1...A_n} [\tau_A_K] \text{ is proportional to a process operator. In this case, let } \sigma_{|\tau_A_K} \text{ be the corresponding correctly normalized process operator. We refer to } \sigma_{|\tau_A_K} \text{ as a conditional process.}

**Definition 8.** (Causal separability) [24]: Every single-node process is causally separable. For \( n \geq 2 \), a process \( \sigma \) on \( n \) quantum nodes \( A_1, ..., A_n \) is said to be causally separable, iff, for any extension of each node \( A_j \) with an additional input system \( \mathcal{H}(A_j^{in}) \) to a new node \( \tilde{A}_j \), defined by \( \mathcal{H}(\tilde{A}_j) := \mathcal{H}(A_j^{in}) \otimes \mathcal{H}(A_j^{in}) \) and \( \mathcal{H}(\tilde{A})_{out} := \mathcal{H}(A_{out}) \), and any auxiliary quantum state \( \rho \in \mathcal{L} (\mathcal{H}(A_i^{in}) \otimes ... \otimes \mathcal{H}(A_n^{in})) \), the process \( \sigma \otimes \rho \) on the quantum nodes \( \tilde{A}_1, ..., \tilde{A}_n \) decomposes as

\[
\sigma \otimes \rho = \sum_{k=1}^{n} q_k \sigma_{(k)}^{out},
\]

with \( q_k \geq 0 \), \( \sum_k q_k = 1 \), where for each \( k \), \( \sigma_{(k)}^{out} \) is a process in which there can be no signalling to \( \tilde{A}_k \) from the rest of the nodes, and where for any CP map \( \tau_{\tilde{A}_k} \) that can take place at the node \( \tilde{A}_k \), the conditional process on the remaining \( n-1 \) nodes, \( \sigma_{(k)}^{out} \tau_{\tilde{A}_k} \), is itself causally separable.

Note that the cyclicity of a QCM does not in general imply causal nonseparability of the process, even in the case that the QCM is faithful. Consider, for example, the quantum SWITCH as described in Sec. [VII] with process operator \( \sigma_{SBF|ABF} \). Tracing out the system \( F^n \), we obtain a reduced 3-node process that (relabelling \( C \) as \( P \)) is both faithful and Markov for the graph of Fig. 11b having the form \( \sigma_{ABP} = \rho_{A|B} \rho_{B|A} \rho_P \). This process is causally separable - it can be understood as describing a situation in which the order between \( A \) and \( B \) depends in an incoherent manner on the logical value of the control qubit prepared at the initial time.

In the case of unitary processes, however, things are much simpler.

**Theorem 4.** A unitary process is causally nonseparable iff it has a cyclic causal structure.

**Proof:** See App. E. \( \square \)

If a unitary process has a causal structure given by an acyclic graph, then it is a unitary comb [57]. Hence a unitary process is either a comb or is causally non-separable. Intermediate possibilities, such as dynamical causal order, cannot arise.

**XI. CYCLICITY AND CLASSICAL PROCESSES**

If a process operator is diagonal in a basis that is a product of local bases for the input and output Hilbert spaces at each node, it is equivalent to a classical process [3] [13] [53], where each node \( X \) is associated with a pair of classical variables \( X^{in} \) and \( X^{out} \). Following Ref. [26] we call such classical nodes classical split nodes. Classical processes are studied in detail in Refs. [12] [36] [53]. (See also Refs. [12] [25].) This section presents the main ideas, and defines (possibly cyclic) classical split-node causal models. For the most part the definitions are the obvious classical analogues of those for the quantum case. While cyclic classical causal models have sometimes been studied (see, e.g., Refs. [68] [71]), for example to encompass the possibility of classical feedback loops, they are not of the split-node variety described here, and are not equivalent.

A classical process, defined over classical split-nodes \( X_1, ..., X_n \), corresponds to a map \( \kappa_{X_1, ..., X_n} : X^{in}_1 \times X^{out}_1 \times \cdots \times X^{in}_n \times X^{out}_n \rightarrow \{0,1\} \), such that \( \sum_{X^{in}_1, X^{out}_1, \cdots, X^{in}_n, X^{out}_n} \kappa_{X_1, ..., X_n} \prod_i P(X^{out}_i | X^{in}_i) = 1 \), for any set of classical channels \( \{P(X^{out}_i | X^{in}_i)\} \). A local intervention at a node \( X \), with output \( k_X \), corresponds to a classical instrument \( P(k_X, X^{out} | X^{in}) \). Given a local intervention at each node, the joint probability distribution over the outcomes is

\[ P(k_{X_1}, ..., k_{X_n}) = \]
\[ \sum_{X_1^{in}, X_1^{out}, \ldots, X_n^{in}, X_n^{out}} \left( \kappa_{X_1, \ldots, X_n} \prod_i P(k_{X_i}, X_i^{out} | X_i^{in}) \right). \]

A special case of a classical process is a deterministic process \( \kappa^f_{X_1, \ldots, X_n} \), for which \( P(X_1^{in}, \ldots, X_n^{in} | X_1^{out}, \ldots, X_n^{out}) = \delta((X_1^{in}, \ldots, X_n^{in}), f(X_1^{out}, \ldots, X_n^{out})) \), where \( f : X_1^{out} \times \ldots \times X_n^{out} \rightarrow X_1^{in} \times \ldots \times X_n^{in} \) is a function. When \( f \) is bijective, we call such a process reversible. It was shown in Ref. [13] that the set of classical processes over nodes \( X_1, \ldots, X_n \) forms a polytope, and that the deterministic polytope, defined as all convex mixtures of deterministic processes, is in general a strict subset of it. While all classical processes on two nodes are causally separable [3], on three or more nodes there exist classical processes, including deterministic classical processes, that are causally nonseparable – an example from Ref. [33] was described in Sec. [VII].

**Definition 9.** (Classical split-node causal model (CSM) – generalized): A CSM is given by:

1. a causal structure represented by a directed graph \( G \) with vertices corresponding to classical split-nodes \( X_1, \ldots, X_n \),
2. for each \( X_i \), a classical channel \( P(X_i^{in} | Pa(X_i)^{out}) \), where \( Pa(X_i) \) denotes the set of parents of \( X_i \) according to \( G \), such that \( \kappa_{X_1, \ldots, X_n} = \prod_i P(X_i^{in} | Pa(X_i)^{out}) \) is a process operator over \( X_1, \ldots, X_n \).

This definition generalizes that of Ref. [35] to include the case of cyclic graphs, and classical split nodes where the input and output variables have different cardinalities. Ref. [36] presents detailed discussion of the relationship between (acyclic) CSMs and standard classical causal models [49, 50].

In the classical case, causal structure (defined for unitary processes in the quantum case) can be defined for deterministic processes.

**Definition 10.** (Causal structure of a deterministic classical process): Given a deterministic process \( \kappa^f_{X_1, \ldots, X_n} \), the causal structure of the process is the directed graph with vertices \( X_1, \ldots, X_n \) and an arrow \( X_i \rightarrow X_j \) whenever \( X_j^{in} \) depends on \( X_i^{out} \) through the function \( f \).

**Definition 11.** (Classical Markov condition – generalized): A process \( \kappa_{X_1, \ldots, X_n} \) is called Markov for a directed graph \( G \) with classical split-nodes \( X_1, \ldots, X_n \) as its vertices iff it admits a factorization of the form \( \kappa_{X_1, \ldots, X_n} = \prod_{i=1}^n P(X_i^{in} | Pa(X_i)^{out}) \), where \( Pa(X_i) \) denotes the set of parents of \( X_i \) according to \( G \).

The following is immediate.

**Proposition 2.** Every deterministic classical process is Markov for its causal structure.

In the case of general – i.e., not necessarily deterministic – classical processes, an account of their relationship to causal structure can be given that again mirrors the quantum case. Let us adopt the provisional approach that causal structure always inheres in deterministic reversible processes (where reversibility here may not be essential, but is assumed to provide a closer analogue to the quantum case in which unitarity is assumed). Then compatibility with a given directed graph can be defined in terms of extension to a reversible deterministic process with latent local noise variables.

**Definition 12.** (Reversible extendibility): A process \( \kappa_{X_1, \ldots, X_n} \) is reversibly extendible iff there exists a reversible deterministic process \( \kappa^f_{X_1, \ldots, X_n, F, \lambda} \) with an additional leaf node \( F \) and root node \( \lambda \), such that \( \kappa_{X_1, \ldots, X_n} = \sum_{\lambda^{in}, \lambda^{out}} P(\lambda^{out}) P(\lambda^{out}) \) for some \( P(\lambda^{out}) \).

**Definition 13.** (Compatibility with a directed graph): A process \( \kappa_{X_1, \ldots, X_n} \) is compatible with a directed graph \( G \) with nodes \( X_1, \ldots, X_n \), iff \( \kappa_{X_1, \ldots, X_n} \) is reversibly extendible to a deterministic process \( \kappa^f_{X_1, \ldots, X_n, F, \lambda_{X_1, \ldots, X_n}} \) with an additional leaf node \( F \), root nodes \( \lambda_i \), and a product distribution \( \prod_i P(\lambda_i^{out}) \), such that through \( f \), \( X_i^{in} \) depends neither on \( \lambda_i^{out} \) for \( j \neq i \) nor on \( X_j^{out} \) for \( X_j \notin Pa(X_i) \) (with \( Pa(X_i) \) referring to \( G \)).

With Prop. 2, the following analogue of Thm. 2 is straightforward.

**Theorem 5.** If a classical process \( \kappa_{X_1, \ldots, X_n} \) is compatible with a directed graph \( G \), then it is also Markov for \( G \).

As in the quantum case, we leave open whether the converse to Thm. 5 holds.

**Conjecture 2.** If a process \( \kappa_{X_1, \ldots, X_n} \) is Markov for a directed graph \( G \), then it is compatible with \( G \).

We remark only that Conjecture 2 is not obviously implied by its quantum counterpart, Conjecture 1. First, it is not known whether reversible extendibility implies unitary extendibility for a classical process when seen as a special case of a quantum process. Second, even if this is the case, it is still conceivable that while a classical process that is Markov for a given graph may admit unitary extensions with the required no-influence properties when viewed as a quantum process, no such extension may be equivalent to a deterministic classical process for the given preferred basis.

We conclude with the following observation.

**Theorem 6.** Given a set of classical split nodes \( X_1, \ldots, X_n \), the set of reversibly extendible classical processes on \( X_1, \ldots, X_n \) coincides with the deterministic polytope.

**Proof:** See App. 11. If Conjecture 2 holds, then Thm. 6 implies in particular that the process defined by a CSM must always belong to the deterministic polytope. An example of
a classical process $\kappa_{X_1 \ldots X_n}$ outside of the deterministic polytope is described in Ref. [13] (and denoted $E_{ex}$ therein). It is not too hard to show that this process is not Markov for any directed graph, hence cannot be the process defined by a CSM, in keeping with Conjecture 2.

XII. CONCLUSIONS

This work presented an extension of the framework of quantum causal models from Refs. [35] [36] to include cyclic causal structures. The extension is the natural generalization of the concepts in the acyclic case and takes the causal model perspective seriously by proposing an alternative view of certain processes. Rather than having an ‘indefinite causal order’, they arise as a result of a definite, but cyclic, causal structure. We showed that the quantum SWITCH, and a process that violates causal inequalities, found by Araújo and Feix and described by Baumeler and Wolf, can be seen as the processes defined by cyclic quantum causal models. We also gave decompositions of any SWITCH-type process and of the unitary extension of the aforementioned process by Araújo and Feix, enabling diagrammatic representations that makes the internal causal structures evident. Applications of these results included proofs that any unitarily extendible bipartite process is causally separable, and that any unitary process is cyclic if and only if it is causally nonseparable. Although we do not provide any details, we note briefly that the generalization of quantum causal models to the cyclic case would also allow an extended version of the causal discovery algorithm sketched in Ref. [36] (inspired in turn by the first of its kind in Ref. [52]) such that cyclic causal structures may be discovered and output by the algorithm.

One of the main questions left open is the validity of our conjecture that Markovianity implies compatibility for cyclic graphs, which would generalize one of the main results established for the acyclic case in Ref. [36]. The validity of this conjecture has consequences, which we spell out as follows.

Ref. [52], in motivating the study of unitary extendibility of processes, includes the suggestion that unitary extendibility should be regarded as a necessary condition for a process to be realizable in nature. Here, the meaning of ‘realizable’ is a little vague, but might be taken, for example, to include exotic scenarios involving gravity as well as the time-delocalized sense discussed above in which some processes have been realized in the laboratory. (It does not include realization via postselection, since it is known that all processes can be realized under a suitable postselection [11] [14] [29] [72].) The suggestion would hold if all processes, once sufficient systems are included, are unitary at the most fundamental level.

Alternatively, under the assumption that the process operator framework provides the most general description of the possible correlation between quantum systems, in non-postselected scenarios, one may speculate that a necessary condition for a process to be realizable in nature is that it can arise from a QCM. Here, ‘arise’ means that there is a QCM with process $\sigma'$ such that $\sigma$ can be obtained from $\sigma'$ by inserting channels at some of the nodes of $\sigma'$ and marginalizing over them. The idea is that any correlations described by such a process admit a causal explanation, albeit one that may involve cycles. On the other hand, any process that cannot arise from a QCM in this manner describes correlations that are not amenable to an understanding in causal terms.

The connection with unitary extendibility is that any process that is unitarily extendible has the property that it can arise from a QCM. Furthermore, if Conjecture 1 holds, then any process that is not unitarily extendible cannot arise from a QCM. Hence if Conjecture 1 holds, the speculation above coincides with the suggestion of Ref. [59].

If Conjecture 1 fails, then there is a peculiar class of cyclic quantum causal models, in which the process is Markov for the graph but not compatible with the graph. We leave open the status of such models, in particular whether any meaning can be given to the arrows of the graph, given that there is no suitable unitary extension to define causal relations, and whether the process might be realizable or not.

Beyond establishing the conjecture, future work might study the extent to which other core results of the framework of quantum causal models in the acyclic case, such as the d-separation theorem [36], can be generalized in an appropriate way to the cyclic case, as has been done for the classical framework (see, e.g., Refs. [70] [71]).

XIII. ACKNOWLEDGMENTS

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Appendix A: Characterisation of process operators

Let \( \{ \eta_k \}_{k=0}^{d_X^2-1} \) denote a Hilbert-Schmidt (HS) basis for \( \mathcal{L}(\mathcal{H}_X) \), i.e., a set of operators such that they are orthonormal with respect to the HS inner product and, in addition, traceless for all \( l = 1, \ldots, d_X^2-1 \), while \( \eta_0 = (1/d_X)I_X \). Any \( \sigma \in \mathcal{L}(\mathcal{H}_A^{in} \otimes \mathcal{H}_B^{in} \otimes \mathcal{H}_A^{out} \otimes \mathcal{H}_B^{out}) \) can be expanded in a HS basis as

\[
\sigma = \sum_{l_1,l_2,l_3,l_4} \alpha_{l_1 l_2 l_3 l_4} \eta_{l_1}^{A^{in}} \otimes \eta_{l_2}^{A^{out}} \otimes \eta_{l_3}^{B^{in}} \otimes \eta_{l_4}^{B^{out}}.
\]

A term of type \( A^{in} \) in the expansion is a summand with non-trivial action only on \( A^{in} \), i.e., \( l_1 \neq 0 \) and \( l_2 = l_3 = l_4 = 0 \). Similarly for types \( A^{out B^{in}} \) etc.

It was shown in Ref. \[3\] that \( \sigma \) being a bipartite process operator is equivalent to \( \sigma \geq 0 \), \( \text{Tr}[\sigma] = 1 \), and that in a HS basis expansion, in addition to a term, which is proportional to the identity operator on all four spaces, only the coefficients of terms of the types \( A^{in}, B^{in}, A^{in}B^{in}, A^{in}B^{out}, A^{out}B^{in}, A^{in}A^{out}B^{in} \) and \( A^{in}B^{in}B^{out} \) may be non-vanishing. These conditions were generalized to \( n \) numbers of parties in Ref. \[7\] and can easily be stated as (1) \( \sigma \geq 0 \), (2) \( \text{Tr}[\sigma] = 1 \), and (3) that in a HS basis expansion the only non-vanishing terms, apart from an overall identity operator, are of a type such that there must be at least one node, say \( A_i \), on whose out-space, \( A_i^{out} \), the action is trivial, but on whose in-space, \( A_i^{in} \), the action is non-trivial.

Equivalent conditions were presented in \[9\] where the projector onto the linear subspace of process operators was defined explicitly, giving a basis-independent characterization.

Appendix B: Proof of Prop. 1

Suppose a bipartite cyclic QCM is given by the (unique) cyclic graph \( G \) with two nodes \( A \) and \( B \) from Fig. 1a and a process \( \sigma_{AB} = \rho_{AB} \rho_{BA} \). Markov for \( G \) it follows that \( \sigma_{AB} = \rho_{AB} \otimes \rho_{BA} \), as both factors act on distinct Hilbert spaces. Now suppose that this is a faithful QCM, i.e., both channels \( \rho_{AB} \) and \( \rho_{BA} \) are signalling channels. One way to see that this contradicts the assumption that \( \sigma_{AB} \) is a valid process is by analyzing the non-vanishing types of terms in an expansion of \( \sigma_{AB} \) relative to a Hilbert-Schmidt product basis (see App. A). If signalling from \( B^{out} \) to \( A^{in} \) is possible in \( \rho_{AB} \), then an expansion of just \( \rho_{AB} \) has to contain a non-vanishing term of type \( A^{in}B^{out} \). Similarly, if signalling from \( A^{out} \) to \( B^{in} \) is possible in \( \rho_{BA} \), then an expansion of \( \rho_{BA} \) has to contain a non-vanishing term of type \( B^{in}A^{out} \). Consequently, \( \sigma_{AB} \) has to contain a non-vanishing term of type \( A^{in}B^{out}B^{in}A^{out} \), which is forbidden for a process operator \([3]\). \( \square \)

Appendix C: Product of commuting operators not necessarily a process operator

In Sec. III it was observed that not all cyclic graphs support a faithful cyclic QCM (see Prop. 1). This Appendix shows that, given a cyclic graph \( G \) that does support a faithful cyclic QCM, it is not true that any product of commuting operators \( \prod_i \rho_{A_i|P_{A_i}(A_i)} \), with parental sets as in \( G \), constitutes a process operator. Consider for instance the graph \( G \) in Fig. 1b (and see Sec. X, where a faithful cyclic QCM over \( G \) is defined). Letting the three nodes \( A, B \) and \( C \) be classical split nodes (see Sec. XI), with classical bits \( A^{in}, A^{out}, B^{in}, B^{out}, C^{in} \) and \( C^{out} \), define classical channels as in Eqs. C1-C2. It is easy to see that the signalling relations through the channels \( P(A^{in}|B^{out},C^{out}) \) and \( P(B^{in}|A^{out},C^{out}) \) are indeed as in Fig. 1b. At the same time, for any choice of probability distribution \( P(C^{in}) \), the product \( P(A^{in}|B^{out},C^{out})P(B^{in}|A^{out},C^{out})P(C^{out}) \) cannot be a classical process: consider an intervention at \( C \) which fixes \( C^{out} \) to be 0, then \( P(A^{in}|B^{out},0)P(B^{in}|A^{out},0) \) is still a product of two signalling classical channels, which (seeing them as special cases of quantum channels) was already established in the proof of Prop. 1 to be in contradiction with being a process. This establishes the claim.

\[
P(A^{in}|B^{out},C^{out}) := \begin{cases} P(0|0,0) = 0.4, & P(0|0,1) = 0.3, & P(0|1,0) = 0.8, & P(0|1,1) = 0.3, \\ P(1|0,0) = 0.6, & P(1|0,1) = 0.7, & P(1|1,0) = 0.2, & P(1|1,1) = 0.7. \end{cases} \tag{C1}
\]
\[ P(B^{\text{in}}|A^{\text{out}},C^{\text{out}}) := \begin{cases} P(0|0,0) = 0.5, & P(0|0,1) = 0.3, & P(0|1,0) = 0.25, & P(0|1,1) = 0.1, \\ P(1|0,0) = 0.5, & P(1|0,1) = 0.7, & P(1|1,0) = 0.75, & P(1|1,1) = 0.9. \end{cases} \] (C2)

Appendix D: Proof of Thm. 3

Suppose the bipartite quantum process operator \( \sigma_{AB} \) is unitarily extendible. Consider an arbitrary unitary extension of it, \( \sigma_{\tilde{A}BFP} = \rho_{\tilde{A}BFP}^{\text{in}} \). From Eq. 8 it follows that the reduced process obtained by tracing out \( F^{\text{in}} \) has the form

\[ \sigma_{ABP} = \text{Tr}_{\text{Fin}}[\rho_{\tilde{A}BFP}^{\text{in}}] = \sum_{i \in I} \rho_{A|B|P_{i}} \otimes \rho_{B|P_{i}} A, \]

for the decomposition \( \mathcal{H}_{\text{pout}} = \bigoplus_{i \in I} \mathcal{H}_{P_{i}} \otimes \mathcal{H}_{P_{i}} \), identified by \( S \), where \( \rho_{A|B|P_{i}} = \text{Tr}_{P_{i}}[\rho_{\tilde{A}B|P_{i}}^{\text{in}}] \) and \( \rho_{B|P_{i}} A = \text{Tr}_{P_{i}}[\rho_{F_{i}B|P_{i}}^{\text{in}}] \) and, where \( \rho_{A|B|P_{i}} \otimes \rho_{B|P_{i}} A \) is taken as an operator on the whole space, acting as zero map on all but the \( i \)th subspace. Note that from \( \sigma_{ABP} \) being a process operator it follows that feeding in any \( \tau_{P} \in \mathcal{L}(\mathcal{H}_{\text{pout}}) \) gives a quantum process operator on the nodes \( A \) and \( B \). Let \( i \in I \) be some fixed index and suppose through the channel \( \rho_{A|B|P_{i}} \) system \( B^{\text{out}} \) can signal to \( A^{\text{in}} \) and similarly, through the channel \( \rho_{B|P_{i}} A \) system \( A^{\text{out}} \) can signal to \( B^{\text{in}} \). Then there exists an appropriate state \( \tau_{P} \), which has only support on the \( i \)th subspace, and which is of a product form \( \gamma_{P_{i}} \otimes \phi_{P_{i}} A \), such that in

\[ \text{Tr}(P_{i}),[\rho_{A|B|P_{i}} \gamma_{P_{i}}] \otimes \text{Tr}(P_{i}),[\rho_{B|P_{i}} A \phi_{P_{i}} A], \] (D1)

both, the marginal channel on the left is signalling from \( B^{\text{out}} \) to \( A^{\text{in}} \) and the one on the right from \( A^{\text{out}} \) to \( B^{\text{in}} \). Since the expression in Eq. (D1) has to give a process operator over \( A \) and \( B \), this yields a contradiction due to Prop. Hence, for each \( i \) at most one of the channels \( \rho_{A|B|P_{i}} \) and \( \rho_{B|P_{i}} A \) allow signalling from \( B^{\text{out}} \) to \( A^{\text{in}} \) or from \( A^{\text{out}} \) to \( B^{\text{in}} \), respectively. By assumption there exists an appropriate \( \tau_{P} \in \mathcal{L}(\mathcal{H}_{\text{pout}}) \) such that

\[ \sigma_{AB} = \sum_{i} \text{Tr}(P_{i}),\left[ (\rho_{A|B|P_{i}} \otimes \rho_{B|P_{i}} A) \tau_{P} \right]. \] (D2)

By the above analysis, it also follows that each summand in Eq. (D2) has to be a process operator up to normalization. Since they sum up to a process operator, the inverses of the normalization constants have to form a probability distribution and one can therefore write \( \sigma_{AB} = \sum_{i} \rho_{i} \sigma_{AB}^{(i)} \), where each \( \sigma_{AB}^{(i)} \) is a process operator with at most \( A \) signalling to \( B \) or vice versa. This is the form of a bipartite causally separable process operator.

Note further that if \( \rho_{A|B|P_{i}} \) is non-signalling from \( B^{\text{out}} \) to \( A^{\text{in}} \), then in \( V_{i} \) there is no influence from \( B^{\text{out}} \) to \( A^{\text{in}} \), and similarly, if \( \rho_{B|P_{i}} A \) is non-signalling from \( A^{\text{out}} \) to \( B^{\text{in}} \), then in \( W_{i} \) there is no influence from \( A^{\text{out}} \) to \( B^{\text{in}} \). Therefore, the above constraints mean that each term \( V_{i} \otimes W_{i} \) in Eq. 8 corresponds to a process over nodes including \( A \) and \( B \) that allows signalling in at most one direction between \( A \) and \( B \). The latter always admits an implementation as a unitary circuit fragment with nodes \( A \) and \( B \) in a fixed order. Since the full unitary \( U \) of the unitary extension is a direct sum of such fixed-order unitary processes taking place in the different orthogonal subspaces, and every operation at the nodes \( A \) and \( B \) can be dilated to a unitary, the full unitary process \( \sigma_{ABFP} = \rho_{\tilde{A}BFP}^{\text{in}} \) can be realized by coherently conditioning which of the corresponding fixed-order unitary circuits takes place on the logical value of some control \( n \)-level quantum system, where \( n \) is the number of different subspaces. Note that since the systems involved in the fixed-order circuits may have different dimensions, this implementation in practice may require ‘bringing in’ different systems depending on the control variable \( i \), but this can always be seen as part of a process on a larger system of a fixed dimension. Moreover, the fixed-order processes in the different orthogonal subspaces can be grouped into two sets: one in which \( A \) is before \( B \) and another one in which \( B \) is before \( A \). This allows embedding the process into another one where one of two possible circuits (in which \( A \) and \( B \) occur in different orders) is applied in a coherently controlled fashion based on the logical value of a control qubit, similarly to the quantum SWITCH. This yields another possible unitary extension \( \sigma_{\tilde{A}BFP} \) of the original bipartite process, where \( \tilde{F}^{\text{in}} \) and \( P^{\text{out}} \) would contain \( F^{\text{in}} \) and \( P^{\text{out}} \), respectively, as subspaces. The originally assumed unitary extension \( \sigma_{ABFP} \) can then be seen to take place effectively as part of \( \sigma_{\tilde{A}BFP} \).

Appendix E: Proof of Thm. 4

The proof below will use the following two concepts. First, generalizing the notion of a process being unitary from Def. 1, a process is called *isometric* if its induced channel from the output systems of all nodes to the input systems of all nodes arises from an isometry. Second, a *quantum comb*, as defined in Ref. 67 (provided first input and last output system are trivial), is a special kind of quantum process: a process \( \sigma_{A_{1}...A_{n}} \) over

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8After completing this work, we came to know that this result was obtained independently by a different route by Wataru Yokojima, Marco Túlio Quintino, Akihito Soeda and Mio Murao, which has appeared in Ref. 16 since the first preprint of this paper in Ref. 13.
Thus, indexed by (entangled bipartite states, such that every pair of nodes $A_i$ tangled state, shared between node $A_i$ and node $A_j$, Hence, there exists one node, let this be $\tilde{A}_1$ (for an appropriate relabeling), such that $\tilde{A}_2, \ldots, \tilde{A}_{n+1}$ cannot signal to $\tilde{A}_1$ and for all CP maps $\tau_{\tilde{A}_1}$ at that node the conditional process $\tilde{\sigma}|_{\tilde{\tau}_{\tilde{A}_1}}$ is causally separable. Now consider a CP map such that $\tau_{\tilde{A}_1} = |\tau_{\tilde{A}_1}\rangle\langle\tau_{\tilde{A}_1}|$ itself is a rank-1 projector. The process operator $\tilde{\sigma}|_{\tilde{\tau}_{\tilde{A}_1}}$ then still is proportional to a rank-1 projector and, hence, representing an isometric process on the remaining $n$ nodes $\tilde{A}_2, \ldots, \tilde{A}_{n+1}$. As argued above it also is causally separable. By assumption then such an isometric, causally separable process $\tilde{\sigma}|_{\tilde{\tau}_{\tilde{A}_1}}$ on $n$ nodes is a quantum comb.

Notice first that if there is no signalling to $\tilde{A}_1$ from all other nodes in the extended process $\tilde{\sigma}$, then there is no signalling to $A_1$ from all other nodes in the original process $\sigma$. Consider $\tau_{A_1} = |\tau_{A_1}\rangle\langle\tau_{A_1}|$, where $|\phi\rangle\langle\phi|$ is some fixed projector on the ancillary input system $\{A_1\}^{\text{in}}$ and $\tau_{A_1} = |\tau_{A_1}\rangle\langle\tau_{A_1}|$ has rank-1. Since projecting the ancillary systems via $|\phi\rangle\langle\phi|$ leaves the ancillary systems on the remaining nodes in some pure state $|\Phi\rangle\langle\Phi|$, the conditional process on the remaining nodes has the form $\sigma|_{\tau_{A_1}}\otimes|\Phi\rangle\langle\Phi|$. Since the latter is a quantum comb for every $|\Phi\rangle\langle\Phi|$, so must be $\sigma|_{\tau_{A_1}}$.

There are $n!$ different possible total orders of the nodes, given by $A_{\pi(2)}, \ldots, A_{\pi(n+1)}$ for $\pi$ being one of the $n!$ different permutations of $2, \ldots, n + 1$. We will now show (by proof of contradiction) that there exists a reordering $A_{\pi(2)}, \ldots, A_{\pi(n+1)}$ with which the quantum comb $\sigma|_{\tau_{A_1}}$ is compatible for any choice of $|\tau_{A_1}\rangle\langle\tau_{A_1}|$. Suppose there does not exist one such appropriate total order. Then for every permutation $\pi$, there exists $\tau_{A_1}^\pi := |\tau_{A_1}\rangle\langle\tau_{A_1}|$, such that the corresponding quantum comb $\sigma|_{\tau_{A_1}^\pi}$ is incompatible with the total order of the remaining nodes defined by $\pi$. Let $C_l^{\pi}(\sigma) = 0$ for $l = 1, \ldots, n$ be the linear constraint corresponding to the $l$th condition in Eq. (E1) for a process operator $\sigma$ over $n$ nodes to be a valid quantum comb for the total order $\pi$.

Consider a process operator $\tilde{\sigma} := \sum_{\pi=1}^{n!} q_{\pi} \sigma|_{\tau_{A_1}^\pi}$, where $q_{\pi} \geq 0$, $\forall \pi$, and $\sum_{\pi} q_{\pi} = 1$ (letting $\pi$, both, be a permutation as well as an index enumerating those permutations). By construction, for every $\pi$ at least one of the conditions in $\{C_l^{\pi}(\sigma)|_{\tau_{A_1}^\pi} = 0\}_{l=1}^{n}$ fails. Therefore, one can then choose the weights $q_{\pi}$ such that for every $\pi$ the process operator $\tilde{\sigma}$ violates at least one of these constraints $\{C_l^{\pi}(\tilde{\sigma}) = 0\}_{l=1}^{n}$, establishing that $\tilde{\sigma}$ is not a quantum comb for any possible order of the $n$ nodes. More precisely, the condition that $\tilde{\sigma}$ respects the constraints $\{C_l^{\pi}(\tilde{\sigma}) = 0\}_{l=1}^{n}$, for a given $\pi$ can be written as $\sum_{\alpha=1}^{n!} q_{\alpha} C_l^{\pi}(\sigma)|_{\tau_{A_1}^\pi} = 0$ for $l = 1, \ldots, n$, which implies that $(q_1, \ldots, q_{n!})$, viewed as a point in an $(n!)$-dimensional Euclidean space, must belong to a specific
hyperplane in that space. Our assumption that at least one of \(C_{\tilde{\tau}}(\sigma|_{\tau_A^1})\) must be nonzero, makes it a proper hyperplane. Then, in order for \(\tilde{\sigma}\) to be compatible with the quantum-comb conditions for at least one \(\tau\), the point \((q_1, \ldots, q_n)\) must belong to the union of the hyperplanes corresponding to the different values of \(\tau\). Since this is a finite set of hyperplanes, it is possible to find (a continuum of) points in the positive orthant that are outside of this union. Since rescaling \((q_1, \ldots, q_n)\) by a constant factor, which amounts to rescaling \(\tilde{\sigma}\) by a constant factor, does not change the fact of whether any of the above constraints is violated or not, there exists a \((q_1, \ldots, q_n)\) with the required properties, such that \(\tilde{\sigma}\) is not a quantum comb for any total order \(\tau\).

We will now use this fact to construct the contradiction with the assumption that there is no single order \(\pi\) with which all isometric quantum combs \(\sigma|_{\tau_A^1}\) are compatible. To this end, we will first show that, starting from our extended process \(\tilde{\sigma} = \sigma \otimes |\Phi\rangle\langle\Psi|\), for any \(j \in \{2, \ldots, n + 1\}\) it is possible to apply a suitable CP map \(\tau|_{\tau_A^1}\), such that this yields a conditional process of the form \(\tilde{\sigma}|_{\tau_A^1} = [\tilde{\sigma}]_j\langle\tilde{\sigma}|_{\tau_A^1}\otimes|\Phi\rangle\langle\Phi|_{\text{rest}^\tau_{\Delta^1}},\) where \([\tilde{\sigma}]_j = \sum_{j=1}^{n+1} \sqrt{\epsilon_j} \langle\tilde{\sigma}|_{\tau_A^1}\otimes|\Phi\rangle_{\text{rest}^\tau_{\Delta^1}}\) with, recalling Eq. \(E2\), \(\mathcal{H}_{A_j}\) the factor of \(\mathcal{H}_{(A^j)\text{in}}\) sharing the state \(|\phi^\tau\rangle\rangle_{\text{in}}\) with \(\mathcal{H}_{A_1}\), of the node \(A_1\) and \(|\sigma_{\tau_A^1}\rangle\langle\sigma_{\tau_A^1}| = \sigma|_{\tau_A^1}\rangle\langle\sigma_{\tau_A^1}|\), the conditional process on the remaining \(n\) of the original \(n + 1\) nodes, and where \(|\phi\rangle\langle\phi|_{\text{rest}^\tau_{\Delta^1}}\) is some pure state on the remaining auxiliary input systems (i.e. \(|\phi\rangle\langle\phi|_{\text{rest}^\tau_{\Delta^1}}\) is in \(\bigotimes_{i\neq j} \mathcal{H}_{(A^i)\text{in}}\) ‘excluding’ the subfactor \(\mathcal{H}_{A_j}\)).

To see this, let \(j \neq 1\). If we apply a CP map of the form \(|\tau\rangle\langle\tau|_{\tilde{\tau}_A^1} = |\chi\rangle\langle\chi|_{\sigma_{\tau_A^1}}\otimes|\phi\rangle\langle\phi|_{\text{rest}^\tau_{\Delta^1}},\) where \(|\chi\rangle = \sum_{j=1}^{n+1} \sqrt{\epsilon_j} \langle\sigma|_{\tau_A^1}\otimes|\Phi\rangle_{\text{rest}^\tau_{\Delta^1}}\) is some projector on the remaining ancillary input systems in \((A^j)\text{in}\), then we will obtain a conditional process of the form \(\tilde{\sigma}|_{\tau_A^1} = [\sigma_j]\langle\sigma_j|_{\tau_A^1}\otimes|\phi\rangle\langle\phi|_{\text{rest}^\tau_{\Delta^1}}\), with \([\sigma_j] = \sum_{\tau=1}^{n+1} \sqrt{\epsilon_j} \langle\sigma|_{\tau_A^1}\otimes|\Phi\rangle_{\text{rest}^\tau_{\Delta^1}}\), where \(\gamma_{\tau} = \text{Tr}(|\tau\rangle\langle\tau|_{\tilde{\tau}_A^1}|\sigma\rangle_{\tau_A^1})\) is a reversibly extendible process on the remaining \(n\) nodes, the trace over which gives \(\prod_{j=2}^{n+1} d_{A^j}\). By our main assumption, the \(n\)-node process \(\tilde{\sigma}|_{\tau_A^1} = [\sigma_j]\langle\sigma_j|_{\tau_A^1}\otimes|\phi\rangle\langle\phi|_{\text{rest}^\tau_{\Delta^1}}\) must be a quantum comb, and since \(|\phi\rangle\langle\phi|_{\text{rest}^\tau_{\Delta^1}}\) is just a state on some input systems, \([\sigma_j]\langle\sigma_j|\) must also be a quantum comb (on the nodes \(A_i \neq A_j\), \(i \neq j\), and the node \(A_j\) extended via the ancillary input system \(a_j\)). But tracing out the system \(a_j\) from the latter quantum comb must also yield a quantum comb on the nodes \(A_i \neq A_j\), which can easily be seen from the quantum-comb conditions. However, by construction, \(\text{Tr}_{a_j}[\sigma_j]\langle\sigma_j| = \tilde{\sigma}\), where \(\tilde{\sigma}\) is not supposed to be a quantum comb, which is a contradiction.

Therefore, there must exist a total order \(\tilde{\pi}\), such that \(\sigma|_{\tau_A^1}\) is a quantum comb compatible with \(\tilde{\pi}\) for every rank-1 \(\tau_A^1\). By the convexity of the set of \(n\)-node operators that are quantum combs compatible with \(\tilde{\pi}\), this automatically extends to all CP maps \(\tau_A^1\).

So far we have shown that the process \(\sigma\) is such that there is a node \(A_1\) to which the rest of the nodes cannot signal, and the remaining nodes can be put in a total order \(A_2, \ldots, A_{n+1}\), such that for every CP map \(\tau_A^1\), the conditional process \(\sigma|_{\tau_A^1}\) is a quantum comb compatible with that order. Now observe that this implies that the full process \(\sigma\) is a quantum comb compatible with the total order \(A_1, A_2, \ldots, A_{n+1}\). Since for all possible CP maps \(\tau_A^1\), it holds that \(\mathcal{C}_l(\sigma|_{\tau_A^1}) = 0\) for \(l = 2, \ldots, n + 1\), it follows from the linearity of these constraints, that the corresponding quantum comb conditions hold for \(\sigma\), i.e. \(\mathcal{C}_l(\sigma) = 0\) holds follows from just \(\sigma\) being a process, since it is equivalent to that if in \(\sigma\) we trace out all of the nodes \(A_2, \ldots, A_{n+1}\), we should be left with, up to normalization, a valid single-node process on \(A_1\). Therefore, the isometric process \(\sigma\) on \(n + 1\) nodes is a quantum comb, too, which completes the proof of Lem. 1 and thereby also that of Thm 4. \(\square\)

Appendix F: Proof of Thm. 6

First, suppose \(\kappa_{X_1 \ldots X_n}\) is a reversibly extendible process, that is, there exists a reversible deterministic process \(\kappa_{X_1 \ldots X_n} = \kappa_{X_1 \ldots X_n, \lambda, \Phi}\) for some bijection \(g : X_1^{\text{out}} \times \ldots \times X_n^{\text{out}} \rightarrow X_1^{\text{in}} \times \ldots \times X_n^{\text{in}} \times F^{\text{in}}\), such that

\[
\kappa_{X_1 \ldots X_n} = \sum_{\lambda^{\text{out}}, \Phi^{\text{in}}} \kappa_{X_1 \ldots X_n, \lambda, \Phi}(\lambda^{\text{out}})
\]

for some probability distribution \(P(\lambda^{\text{out}})\). It follows from the fact that \(\kappa_{X_1 \ldots X_n} = \kappa_{X_1 \ldots X_n, \lambda, \Phi}\) is a classical process that marginalization as in Eq. \(F1\) has to yield a classical process over nodes \(X_1, \ldots, X_n\) for arbitrary distributions \(P(\lambda^{\text{out}})\), in particular for every point-distribution. Hence, for every value \(\lambda\) of \(\lambda^{\text{out}}\), the induced function \(g_{\lambda}(\ldots) = g(\ldots, \lambda)\) has to define a deterministic process for \(n + 1\) nodes and furthermore, also once marginalizing over \(F\) it still has to be a deterministic process for the nodes \(X_1, \ldots, X_n\). Hence, Eq. \(F1\) can be read as establishing that the given \(\kappa_{X_1 \ldots X_n}\) is a convex mixture of deterministic processes over the nodes \(X_1, \ldots, X_n\), i.e. \(\kappa_{X_1 \ldots X_n}\) lies in the deterministic polytope.

Conversely, suppose \(\kappa_{X_1 \ldots X_n}\) lies inside the deterministic polytope, that is, there exists a family of deterministic processes \(\{\kappa_{X_1 \ldots X_n}^f\}_{i=1}^m\) defined by the functions \(f_i : X_1^{\text{out}} \times \ldots \times X_n^{\text{out}} \rightarrow X_1^{\text{in}} \times \ldots \times X_n^{\text{in}}\) such that

\[
kappa_{X_1 \ldots X_n} = \sum_{i=1}^m q_i \kappa_{X_1 \ldots X_n}^f\]

for some probability distribution \(\{q_i\}\). The proof will proceed by first observing that such a process can be seen to arise from one single deterministic process on \(n + 2\) nodes. Together with the fact that every deterministic process is reversibly extendible, proven in Ref. 12, this establishes the claim.
In order to see that indeed an appropriate deterministic process on $n+2$ nodes exists, let $\lambda^{\text{out}}$ and $F^{\text{in}}$ be variables with cardinality $m$ and define the function

$$f : X^{\text{out}} \times \lambda^{\text{out}} \rightarrow X^{\text{in}} \times F^{\text{in}}$$

$$(x, i) \mapsto (f_i(x), i),$$

where $X^{\text{out}} = X_1^{\text{out}} \times ... \times X_n^{\text{out}}$ (similarly for $X^{\text{in}}$) and $x = (x_1, ..., x_n)$. Together with setting $P(\lambda^{\text{out}} = i) := q_i$, $f$ defines a deterministic classical process over the nodes $X_1, ..., X_n$, $\lambda$ and $F$, which gives back $\kappa_{X_1,...,X_n}$ upon marginalization over $\lambda$ and $F$. That $f$ indeed defines a process follows from the fact that arbitrary variation of the distribution $P(\lambda^{\text{out}})$ corresponds to an arbitrary weighting $\{q_i\}$ in the originally given mixture, each case of which has to be a classical process. This concludes the proof. □