

Fully Quantum Inflation: Quantum Marginal Problem Constraints in the Service of Causal Inference

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Consider the problem of deciding, for a particular multipartite quantum state, whether or not it is realizable in a quantum network with a particular causal structure. This is a fully quantum version of what causal inference researchers refer to as the problem of causal discovery. In this work, we introduce a fully quantum version of the inflation technique for causal inference, which leverages the quantum marginal problem. The primary example by which we illustrate the utility of this method is testing compatibility of tripartite quantum states with the quantum network known as the triangle scenario. We show, in particular, how the method yields a complete classification of pure three-qubit states into those that are and those that are not compatible with the triangle scenario. We also provide some illustrative examples involving mixed-states and some where one or more of the systems is higher dimensional. Furthermore, we examine the question of when the incompatibility of a multipartite quantum state with a causal structure can be inferred from the incompatibility of a joint probability distribution induced by implementing measurements on each subsystem. Finally, we present a family of networks, which includes the triangle scenario as a special case, for which causal compatibility constraints can be derived.

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I. INTRODUCTION

By providing a method for formalizing intuitive or explicit cause-effect relationships between variables, causal modeling has become an active subfield of statistics and machine learning [1]. More recently, notions of causality have begun to play an instructive role also in quantum physics. One of the best clues for deducing the precise manner in which quantum physics implies a departure from the principles underlying classical physics, Bell's theorem [2,3], admits a distinctly causal interpretation [4,5]. This newfound interest in the intersection of causality and quantum physics has led to a better understanding of quantum-classical gaps in an array of causal structures [6], the investigation of potential benefits for causal inference [7,8], and the formalization of the notion of an intrinsically quantum causal model [9–11].

In a classical causal model [12,13], a causal structure is represented by a directed acyclic graph (DAG) where each node of the DAG represents a random variable and each directed edge represents a potential causal influence between these. The parameters of the model can be taken to be a set of conditional probability distributions, one for each variable conditioned on its causal parents in the DAG. A given probability distribution over the subset of observed variables is said to be *compatible* with the causal structure if it can be obtained from some choice of the parameters after marginalizing over the unobserved (i.e., latent) variables. A central problem in classical causal inference, which we term the *causal compatibility problem*, is deciding whether a given distribution over observed variables is compatible with a given causal structure.

In this work, we are interested in a fully quantum version of the latter problem, where the distribution over observed variables is replaced by a quantum state over a multipartite quantum system. That is, we are interested in the question: for a given quantum state on a multipartite system, is it compatible with a particular causal structure holding among the subsystems?

To make this question more precise, it is necessary to review the quantum generalization of the notion of a causal model. In a *quantum* causal model [9], a causal structure is still represented by a DAG, but now each node of the DAG

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represents a quantum system. The parameters of the model can be taken to be a set of quantum channels, one for each quantum system where the output of the channel is that quantum system and the inputs are the quantum systems that are its causal parents in the DAG. Here, the distinction between visible and latent systems is best understood as the visible nodes being the ones that are probed in a quantum experiment. If the visible quantum systems under consideration are such that there is no cause-effect relationship holding among any of them, then one can assign a joint quantum state to the visible systems [14]. This is the case we consider here. A given joint quantum state on the visible systems is said to be *compatible* with the causal structure if it can be obtained from some choice of the parameters after marginalizing (i.e., taking the partial trace) over the latent quantum systems.

The problem we address, which we term the *fully quantum causal compatibility problem* is that of deciding whether a given quantum state over the visible systems is compatible with a given causal structure.

We make use of a method known as the inflation technique [15], the first applications of which were focused on the case where the visible nodes are classical, and where the latent nodes can be classical or nonclassical. Here, we apply the technique to the case where both visible and latent nodes are quantum. The inflation technique can be understood at a high level as a method for mapping the problem of determining whether a state on the visible nodes is compatible with a causal structure G to the problem of determining whether a particular set of marginals of the state is compatible with a causal structure G' that is termed an “inflation” of G . More specifically, the *failure* of a solution to the latter problem demonstrates the *incompatibility* of the state with G [16].

In tackling the problem of determining whether a particular set of marginals of the state is compatible with a causal structure G' , one can leverage constraints coming from the marginal problem. For the case of visible nodes that are classical, it is the classical marginal problem that is pertinent, namely, the problem of deciding whether a given set of distributions on various subsets of variables are the marginals of a single joint distribution over all the variables. For the case of visible nodes that are quantum, it is the quantum marginal problem that is pertinent, namely, the problem of deciding whether a given set of *quantum states* on various subsets of quantum systems are the marginals of a single joint quantum state over all the quantum systems.

This connection to the quantum marginal problem means that one can leverage preexisting results in the literature for the purpose of deciding compatibility of quantum states with causal structures having quantum latents. Despite the fact that the quantum marginal problem is known to be difficult in general [17], there has nevertheless been progress in a number of cases. See, e.g., the

thorough list of references in Ref. [18, Sec. 1.2]. Of particular relevance for our purposes are the family of operator inequalities introduced by Hall [19,20] (see also [21]).

The main aim of this work is to showcase the utility of the inflation technique in conjunction with these operator inequalities for questions of compatibility of a joint quantum state with a given causal structure.

For illustrative purposes, we primarily focus on the case of a tripartite system and the well-studied causal structure known as the triangle scenario, i.e., the structure that is depicted in Fig. 1(a). In particular, we use the *Cut inflation* of the triangle scenario [15], depicted in Fig. 1(b). Because the Cut inflation is a so-called *nonfanout* inflation (a notion that will be explained further on), it is applicable in the fully quantum case. Furthermore, for the Cut inflation, it is possible to leverage the marginal problem constraint derived by Hall [19] to obtain strong witnesses of incompatibility.

We will apply the technique for a few different choices of the dimensionalities of the visible quantum systems. We focus on the case of three qubits, but we consider also the case of three qutrits and the case of two qubits and a ququart. We also apply the technique not only to assessments of compatibility of pure-states, but mixed-states as well. Furthermore, we show that it is possible to leverage the same marginal problem constraints to obtain causal compatibility constraints for a range of network causal structures beyond the triangle scenario.

A number of benefits of this approach are worth elucidating here. First, this technique is well suited to numerically specified quantum states. For example, given a state ρ that is specified by experimental state tomography or related methods, it is computationally simple to test compatibility for a specific choice of inflation and marginal inequality. A verdict of incompatibility could then witness the divergence of the actual causal structure of the experiment from the expected one, indicating a deficiency in the experimentalist’s understanding of their setup. This approach is also suitable for considering symbolically specified quantum states, as it utilizes *analytic* quantum marginal problem criteria, in contrast to the semidefinite programming approach of Ref. [22].

One motivation for studying compatibility of pure-states with the triangle scenario (and n -node generalizations thereof where every subset of $n-1$ nodes have a latent common cause acting on them) is the definition of genuine n -partite entanglement proposed in Refs. [22,23], based on entanglement under local operations and shared randomness (LOSR) rather than local operations and classical communication (LOCC) [24]. This definition is distinct from the conventional definition (the one based on biseparability) and overcomes various conceptual problems of the latter, as argued in Ref. [23]. Consider the case of $n = 3$ for simplicity. The LOSR-based definition in this case is that a state is genuine tripartite entangled if it

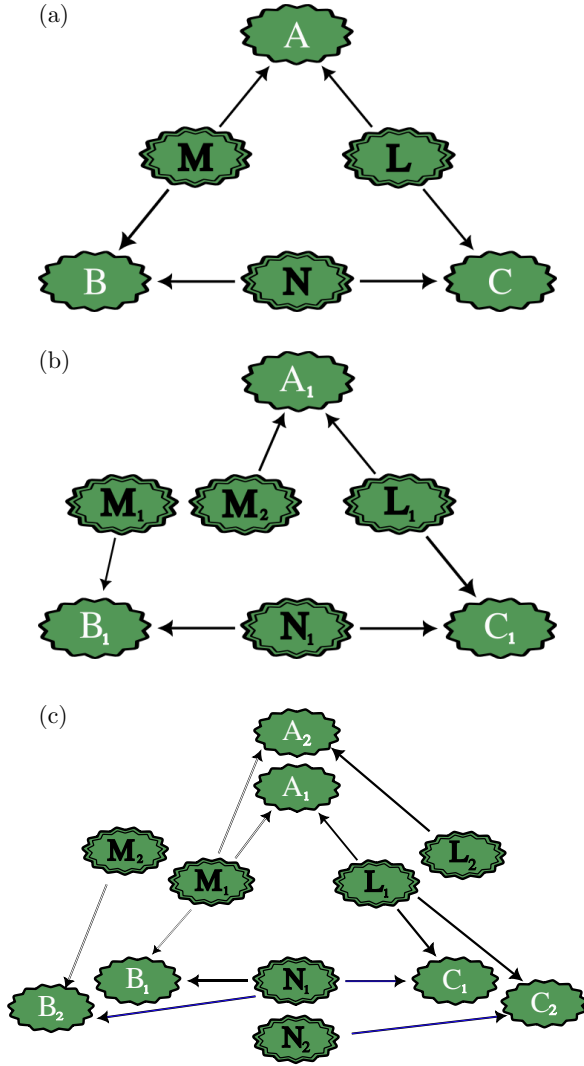


FIG. 1. (a) The directed acyclic graph describing the triangle scenario with quantum semantics for the visible and latent nodes. (b) The AB -Cut inflation of the triangle scenario. (c) The Spiral inflation of the triangle scenario. In all subfigures, visible nodes are indicated by a single-stroke border while latent nodes are indicated by a dual-stroke border. The textured edges and green color of the nodes is to indicate that these are quantum systems rather than classical variables. The convention for the latter is seen in Fig. 2.

cannot be realized by resources of bipartite entanglement. More precisely, it is proposed that a genuine tripartite entangled state is one that cannot be realized by local operations and shared randomness with two-way shared entanglement (LOSR2WSE). If the state to be prepared is *pure*, the shared randomness does not add any additional power [25], so we have that a pure-state is genuinely tripartite entangled when it cannot be realized by local operations with two-way shared entanglement (LO2WSE). But these operations are precisely what can be achieved in the triangle scenario, so a pure-state is genuinely tripartite

entangled when it is incompatible with the triangle scenario. Characterizing the boundary between pure-states that are genuinely tripartite entangled and those that are not, therefore, provides a motivation for characterizing the boundary between pure-states that are compatible with the triangle scenario and those that are not.

The notion of compatibility with the triangle scenario studied here is similar to, but distinct from, the notion of compatibility studied in Ref. [26] (where they refer to the triangle scenario as the *independent triangle network*). This is because the latter article considered only unitaries for the channels mapping the latent systems to the visible systems, rather than allowing arbitrary operations as we do here [27]. That is, Ref. [26] considers state-preparability by local *unitaries* with shared randomness and two-way shared entanglement (LUSR2WSE), while here we consider state-preparability by LO2WSE. When considering the preparability of *pure* multipartite states, which we do in Sec. IV for the triangle scenario, the shared randomness is irrelevant. In such a case, then, the differences between the results of Ref. [26] and our own consists in the differences between state-preparability by LU2WSE and state-preparability by LO2WSE. Because the set of local unitaries is a strict subset of the set of local operations, any state shown to be preparable by LU2WSE is also preparable by LO2WSE, but it is unclear whether or not the opposite implication holds. As such, it is possible that there is a strict inclusion relation between the set of LU2WSE-preparable states and the set of LO2WSE-preparable states. Consequently, any demonstration of incompatibility relative to LU2WSE does not necessarily imply incompatibility relative to LO2WSE. Below, we develop methods that allow for demonstrating the latter type of incompatibility.

The remainder of this article is structured as follows. Section II provides a review of the necessary background on causal models, classical and quantum. Section III reviews the inflation technique for causal inference and shows how to leverage a particular family of operator inequalities related to the quantum marginal problem to derive constraints on compatibility of a quantum state with a causal structure. Application of these new constraints are presented in Secs. IV and V for qubit and higher-dimensional visible nodes respectively, with proofs presented in the appendices. In Sec. VI, we present a family of networks where causal compatibility constraints can be obtained via the methods developed in earlier sections. Section VII discusses avenues for generalizing our results and conclusions.

II. PRELIMINARIES

Throughout this paper, we make frequent reference to directed acyclic graphs (DAGs) as the primary method for representing causal structure [12,13], so it is worthwhile

establishing some of the relevant notation for these DAGs here. DAGs will typically be denoted by the letter G and variations thereof, such as G' . The set of nodes of G will be denoted $\text{Nodes}(G)$ and partitions into two subsets: the visible nodes, denoted $\text{Vnodes}(G)$, and the latent nodes, denoted $\text{Lnodes}(G)$. A DAG G with a partitioning of nodes in this way was termed a *partitioned DAG* in Ref. [28]. All nodes will be labeled by capital letters A, B, C , etc., with letters at the start of the alphabet (A, B, C) usually denoting visible nodes and with letters around the middle (L, M, N) denoting latent nodes. For each node $X \in \text{Nodes}(G)$, $\text{Pa}(X) \subset \text{Nodes}(G)$ denotes the set of parents of X in G , that is, the set of nodes of G for which there is a directed edge from the node to X . Similarly, for each $X \in \text{Nodes}(G)$, $\text{Ch}(X) \subset \text{Nodes}(G)$ denotes the set of children of X in G , that is, the set of nodes of G for which there is a directed edge from X to the node. A node $X \in \text{Nodes}(G)$ is called an *ancestor* of a node $Y \in \text{Nodes}(G)$ if there is a directed path from X to Y in G .

A. Classical causal models

To begin with, consider what is arguably the simplest case: *classical* semantics for both the visible and the latent nodes. In the case of the triangle scenario, this is depicted in Fig. 2. This means that both the visible and the latent nodes are associated with random variables. A joint state on the visible nodes is therefore a joint *probability distribution* over the associated random variables.

Consider a DAG G describing the causal structure. We can also presume that G is in a canonical form wherein latent nodes are necessarily exogenous, that is, they have no parents in G [29].

For a classical causal model, the state on the visible nodes is a joint distribution $P_{\text{Vnodes}(G)}$. To specify a choice of parameter values in the causal model is to specify a distribution over each latent variable, i.e., a set $\{P_L : L \in \text{Lnodes}(G)\}$ (here, the cardinality of the set of values of each L is assumed to be finite but allowed to be arbitrarily

large), and a conditional probability for each visible variable given its causal parents $\{P_{A|\text{Pa}(A)} : A \in \text{Vnodes}(G)\}$ (where the parental sets may include both visible and latent variables) [30].

Definition 1 (Classical G -compatibility of a joint distribution). Consider a joint distribution $P_{\text{Vnodes}(G)}$ over the variables associated with the visible nodes of a causal structure G . We say that $P_{\text{Vnodes}(G)}$ is classically G -compatible if there exists a choice of the parameters in the classical causal model, that is, a choice of $\{P_L : L \in \text{Lnodes}(G)\}$ (distributions on the classical systems associated with the latent nodes) and of $\{P_{A|\text{Pa}(A)} : A \in \text{Vnodes}(G)\}$ (conditional probability distributions defining a stochastic map whose inputs are the classical systems associated with the latent nodes and whose outputs are the classical systems associated with the visible nodes) such that these realize $P_{\text{Vnodes}(G)}$,

$$P_{\text{Vnodes}(G)} = \sum_{L \in \text{Lnodes}(G)} \prod_{A \in \text{Vnodes}(G)} P_{A|\text{Pa}(A)} \prod_{L \in \text{Lnodes}(G)} P_L. \quad (1)$$

where $\sum_{L \in \text{Lnodes}(G)}$ indicates marginalization over the variables assigned to latent nodes.

We now consider the concrete example of the triangle scenario. We use the notation for nodes presented in Fig. 2, that is, the visible nodes are denoted A, B, C and the latent nodes are denoted L, M, N , and the variables associated with these nodes are denoted in the same manner as the nodes themselves. A joint distribution P_{ABC} is compatible with the triangle scenario in a classical causal model if there exists a choice of parameters $P_{A|LM}, P_{B|MN}, P_{C|LN}, P_L, P_M$, and P_N such that

$$P_{ABC} = \sum_{LMN} P_{A|LM} P_{B|MN} P_{C|LN} P_L P_M P_N. \quad (2)$$

B. Quantum causal models

We now consider quantum causal models [9–11], where both the latent and visible nodes have quantum semantics.

In the case of the triangle scenario, this is depicted in Fig. 1(a).

For simplicity, we restrict our attention to causal structures wherein no two visible nodes appear in a cause-effect relationship (i.e., one visible node is never in the causal ancestry of another visible node) and wherein all latent nodes are exogenous (i.e., have no parents in the causal structure). This pair of restrictions together imply that the causal structure has just two layers: a layer of exogenous latent nodes and a layer of visible nodes. Such causal structures are sometimes termed *networks* [5,31] and we shall adopt this terminology here [32].

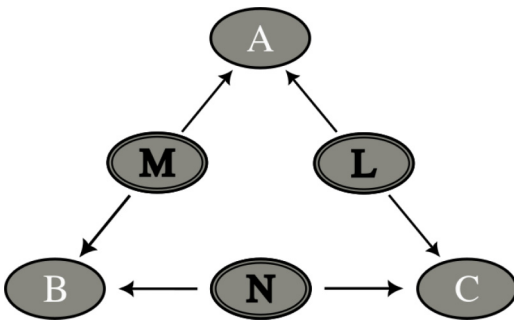


FIG. 2. The directed acyclic graph describing the triangle scenario with classical semantics for the visible nodes, labeled A, B , and C , and the latent nodes, labeled L, M , and N .

In contrast with a classical causal model, which assigns a *variable* to each node (the important aspect of which is the cardinality of its set of values), a quantum causal model assigns a *quantum system* to each node (the important aspect of which is the dimension of Hilbert space associated with it). Consequently, to specify a choice of parameter values in a quantum causal model is to specify two types of parameters: (i) quantum states on the systems associated with the latent nodes (where the dimension of the Hilbert space associated with each latent node is assumed to be finite but allowed to be arbitrarily large) [33] and (ii) quantum channels (i.e., completely positive and trace-preserving linear maps) from these to the quantum systems associated with the visible nodes.

It follows that the entity whose compatibility with a causal structure is to be assessed is no longer a joint probability distribution, but a joint quantum state, specifically, $\rho_{Vnodes(G)}$, i.e., a positive trace-one operator on the Hilbert space $\bigotimes_{A \in Vnodes(G)} \mathcal{H}_A$.

Because of the no-broadcasting theorem in quantum theory [34], if a given latent node influences more than one visible node, one cannot imagine that the state of that node is broadcast to each of the children, as one could classically. The main differences between the definitions of the notion of a quantum causal model proposed in various works, such as Refs. [9–11], relate to how to meet this challenge. However, disagreements about the definition are not relevant to the compatibility problem. This is because the definition of the causal compatibility problem allows the Hilbert spaces associated with the latent nodes to be of arbitrary (finite) dimensionality, and the differences between these approaches arise only when one fixes the dimensionality. We here adopt the following approach: Suppose that the set of visible nodes that are children of a latent node L are denoted $Ch(L)$. Then the Hilbert space associated with the latent node L , $\mathcal{H}_L$, is presumed to factorize into a set of Hilbert spaces indexed by its children. That is, $\mathcal{H}_L = \bigotimes_{A \in Ch(L)} \mathcal{H}_{L(A)}$. The first type of parameter in the causal model is a quantum state ρ_L , i.e., a positive trace-one operator on the space of linear operators on the Hilbert space associated with L , $\rho_L \in \mathcal{L}(\mathcal{H}_L)$. Given the factorization just described, the state ρ_L can be conceptualized as $\rho_{L(A), L(B), \dots, L(Z)} \in \mathcal{L}(\mathcal{H}_{L(A)} \otimes \mathcal{H}_{L(B)} \otimes \dots \otimes \mathcal{H}_{L(Z)})$, where $A, B, \dots, Z \in Ch(L)$. Such a state can clearly describe correlations between the different subsystems of L .

The second type of parameter of the causal model specifies how each visible node depends on its causal parents. For each visible node $A \in Vnodes(G)$, one specifies a quantum channel whose output space is $\mathcal{L}(\mathcal{H}_A)$, the operator space associated with A . Let $Pa(A)$ be defined as $\{L^{(A)} : L \in Pa(A)\}$. That is, for each latent node L among the parents of A , include within $\tilde{Pa}(A)$ only $L^{(A)}$, the subsystem of L that influences A . Thus, whereas $Pa(A)$ describes the collection of latent nodes that are parents of A , $\tilde{Pa}(A)$

describes the collection of *subsystems* of the latent nodes that have an influence on A . The input space of the quantum channel whose output space is $\mathcal{L}(\mathcal{H}_A)$ is $\mathcal{L}(\mathcal{H}_{\tilde{Pa}(A)})$. The channel can consequently be denoted $\mathcal{E}_{A|\tilde{Pa}(A)}$. There is one such channel for each visible node.

We can now define what it means for a joint quantum state on the visible nodes of a network G to be compatible with G for quantum semantics of the latent nodes.

Definition 2 (G-compatibility in quantum causal models). Let G be a network and consider a joint quantum state $\rho_{Vnodes(G)}$ over the systems associated with the visible nodes of G . The state $\rho_{Vnodes(G)}$ is said to be G -compatible with the network G within a quantum causal model if there exist a choice of the parameters of the model that realizes $\rho_{Vnodes(G)}$. More precisely, the joint state $\rho_{Vnodes(G)}$ is G -compatible if, for each latent node $L \in Lnodes(G)$, there exists a choice of quantum state ρ_L , and for each visible node $A \in Vnodes(G)$, there exists a choice of quantum channel $\mathcal{E}_{A|\tilde{Pa}(A)}$, such that

$$\rho_{Vnodes(G)} = \bigotimes_{A \in Vnodes(G)} \mathcal{E}_{A|\tilde{Pa}(A)} \left(\bigotimes_{L \in Lnodes(G)} \rho_L \right). \quad (3)$$

We briefly comment on the choice of having the latent spaces factorize and what that means for the notion of G -compatibility defined above. An alternative choice would be to not assume that latent spaces factorize but instead enforce that the channel parameters $\mathcal{E}_{A|Pa(A)}$ mutually commute on common input spaces. As was demonstrated in Ref. [9], this alternative is well-motivated by a quantum generalization of the notion of common cause in classical causal modeling. However, in the context of quantum causal compatibility, if the latent spaces are finite dimensional (but of arbitrarily large dimension) as we consider here, there is, in fact, no distinction between the factorizing case and the commuting case. That is, any state ρ that is G -compatible with respect to the former notion is also G -compatible with respect to the latter, and vice versa. If the latent spaces are instead infinite dimensional, then the results of, e.g., Refs. [35,36] indicate that there may indeed be a distinction between the factorizing and commuting cases in such a scenario. For our present purposes, we consider finite (but arbitrary large) dimension of latent spaces only, which can be understood as defining the scope of application of the techniques developed below.

To better understand the notion of G -compatibility in a quantum causal model, it is worthwhile once more to consider the concrete example of the triangle scenario, using the notational convention of Fig. 1(a). In this case, the Hilbert spaces of each latent node factorize into a pair of subspaces, i.e., $\mathcal{H}_L \cong \mathcal{H}_{L(A)} \otimes \mathcal{H}_{L(C)}$, $\mathcal{H}_M \cong \mathcal{H}_{M(A)} \otimes \mathcal{H}_{M(B)}$, $\mathcal{H}_N \cong \mathcal{H}_{N(B)} \otimes \mathcal{H}_{N(C)}$. A quantum state ρ_{ABC} on $\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C$ is *triangle-compatible* if

there exist quantum states of the latent nodes $Q_L = Q_{L^{(A)}L^{(C)}}$, $Q_M = Q_{M^{(A)}M^{(B)}}$, and $Q_N = Q_{N^{(B)}N^{(C)}}$ and quantum channels $\mathcal{E}_{A|L^{(A)}M^{(A)}} : \mathcal{H}_{L^{(A)}} \otimes \mathcal{H}_{M^{(A)}} \rightarrow \mathcal{H}_A$, $\mathcal{E}_{B|M^{(B)}N^{(B)}} : \mathcal{H}_{M^{(B)}} \otimes \mathcal{H}_{N^{(B)}} \rightarrow \mathcal{H}_B$, and $\mathcal{E}_{C|L^{(C)}N^{(C)}} : \mathcal{H}_{L^{(C)}} \otimes \mathcal{H}_{N^{(C)}} \rightarrow \mathcal{H}_C$ such that [37]

$$\rho_{ABC} = \mathcal{E}_{A|L^{(A)}M^{(A)}} \otimes \mathcal{E}_{B|M^{(B)}N^{(B)}} \otimes \mathcal{E}_{C|L^{(C)}N^{(C)}}(Q_{L^{(A)}L^{(C)}} \otimes Q_{M^{(A)}M^{(B)}} \otimes Q_{N^{(B)}N^{(C)}}). \quad (4)$$

As an aside, note that the partitioning of the latent systems into subsystems, each of which influences a different child node of the latent node, also provides an alternative way of defining a classical causal model. Take the triangle scenario as an example. The parametrization of the classical causal model that we provided earlier was $P_{A|LM}$, $P_{B|MN}$, $P_{C|LN}$, P_L , P_M , and P_N such that

$$P_{ABC} = \sum_{LMN} P_{A|LM} P_{B|MN} P_{C|LN} P_L P_M P_N. \quad (5)$$

However, one can also partition each latent variable into a pair of latent variables and make each child depend on just one element of the pair. For instance, one defines $L = (L^{(A)}, L^{(C)})$ and one makes A depend only on $L^{(A)}$ and C depend only on $L^{(C)}$. The parametrization of the classical causal model we obtain in this way is $P_{A|L^{(A)}M^{(A)}}$, $P_{B|M^{(B)}N^{(B)}}$, $P_{C|L^{(C)}N^{(C)}}$, $P_{L^{(A)}L^{(C)}}$, $P_{M^{(A)}M^{(B)}}$, and $P_{N^{(B)}N^{(C)}}$ such that

$$P_{ABC} = \sum_{LM,N} P_{A|L^{(A)}M^{(A)}} P_{B|M^{(B)}N^{(B)}} P_{C|L^{(C)}N^{(C)}} \times P_{L^{(A)}L^{(C)}} P_{M^{(A)}M^{(B)}} P_{N^{(B)}N^{(C)}}. \quad (6)$$

This second parametrization is clearly subsumed as a special case of the first. To see that the first is also subsumed as a special case of the second, it suffices to note that one can take $L^{(A)}$ and $L^{(C)}$ to be two copies of the L of the first model and to take the distribution over $L^{(A)}L^{(C)}$ to be what one obtains from the distribution P_L by applying a copy operation, so that $P_{L^{(A)}L^{(C)}} = P_L \delta_{L^{(A)},L} \delta_{L^{(C)},L}$. A similar observation holds for any causal structure.

This demonstrates that one can recover a classical causal model from a quantum causal model by particularizing to density operators that are diagonal in some fixed product basis over the subsystems, since these are equivalent to probability distributions, and channels that act as stochastic maps relative to these bases, since these are equivalent to conditional probability distributions.

III. FULLY QUANTUM INFLATION

A. A description of the technique

The inflation technique for causal inference [15] provides a method for resolving questions of causal compatibility. This method was inspired by ideas from the

literature on Bell's theorem, namely, derivations of Bell's theorem that leverage results from the classical marginal problem.

At a high level, the inflation technique can be conceptualized as a means for converting facts about a marginal problem into facts about causal compatibility. We explore a particular version of this problem in the present paper, namely, how to make use of facts about the quantum marginal problem to obtain conclusions about causal compatibility between a causal structure and a joint quantum state.

In the following, we will generalize the inflation technique to the case of quantum causal models. Note that previous work allowed the *latent nodes* to be quantum, but a description of the inflation technique for the case where the *visible nodes* are quantum has not been provided previously. It is worth noting a subtlety regarding terminology at this point. Whether a causal model is termed “classical” or “quantum” refers to whether all the nodes are classical or all are quantum. The term “quantum inflation,” on the other hand, has been used [31] to describe the inflation technique wherein the latent nodes are quantum but the visible nodes are still classical (and in particular the case where one can treat fanout inflations). One consequently cannot refer to the inflation technique applied to quantum causal models as simply “quantum inflation.” Therefore, we introduce the term “fully quantum inflation” to refer to the technique when both the latent and the visible nodes are quantum.

It is useful to contrast the classical and quantum cases. We will not, however, review the inflation technique for classical causal models. Rather, we will present the technique only for quantum causal models. The description of the technique for classical causal models can be recovered from the quantum one, as noted at the end of Sec. IIB, by simply restricting attention to density operators that are diagonal in some fixed product basis over the subsystems and channels that act as stochastic maps relative to these bases.

The first step in using the inflation technique consists of producing, from the original DAG G , a new DAG G' , termed the *inflation* of G , in the following way (the reader is referred to Ref. [15] for a more complete treatment). The set of nodes of G' , denoted $\text{Nodes}(G')$, are labeled in such a way that each can be associated with a node of G , with the possibility that more than one node of G' is associated with a single node in G . That is, the inflation G' comes with a fixed surjective map $\text{DropCopyIndex}_{G' \rightarrow G} : \text{Nodes}(G') \rightarrow \text{Nodes}(G)$. If the nodes of G are labeled as $A, B, \dots, Z$, then the nodes of G' can be labeled as $A_i, B_j, \dots, Z_k$, where i, j and k are indices in the natural numbers whose ranges depend on the choice of G' . The surjective map is then defined via $\text{DropCopyIndex}_{G' \rightarrow G}(A_i) = A$ for all i and similarly for the other nodes. We refer to the nodes A_i of G' that are

associated with a given node A of G as *copies* of the latter, and the subscript i is referred to as the *copy-index*.

For certain subsets of nodes of G' and of G , the restriction of the map $\text{DropCopyIndex}_{G' \rightarrow G}$ to these subsets forms a bijection. Suppose that $\mathbf{X} \subseteq \text{Nodes}(G)$ and $\mathbf{X}' \subseteq \text{Nodes}(G')$ are such that, for every $A \in \mathbf{X}$ there is precisely one value of i such that $A_i \in \mathbf{X}'$. In such a case, the restriction of $\text{DropCopyIndex}_{G' \rightarrow G}$ to $\mathbf{X}'$ forms a bijection between $\mathbf{X}'$ and $\mathbf{X}$, and we write $\mathbf{X} \sim \mathbf{X}'$. This bijection can be considered as capturing “sameness of the labels of the nodes up to the identity of the copy-index” (where no copy-index is considered to be one possible choice).

Furthermore, for certain choices of G' , $\mathbf{X}' \in \text{Nodes}(G')$ and $\mathbf{X} \in \text{Nodes}(G)$ such that $\mathbf{X} \sim \mathbf{X}'$, the bijection can be considered to be structure-preserving in the following sense. For a given graph G and a subset $\mathbf{X} \in \text{Nodes}(G)$, we denote by $\text{SubDAG}_G(\mathbf{X})$ the sub-DAG of G consisting of those nodes of G contained in $\mathbf{X}$ and those directed edges of G that connect pairs of nodes within $\mathbf{X}$ [analogous notation is used for G' and $\mathbf{X}' \in \text{Nodes}(G')$]. We then say that the map $\text{DropCopyIndex}_{G' \rightarrow G}$ is a structure-preserving bijection between $\text{SubDAG}_{G'}(\mathbf{X}')$ and $\text{SubDAG}_G(\mathbf{X})$ if the restriction of $\text{DropCopyIndex}_{G' \rightarrow G}$ to $\mathbf{X}'$ is a bijection between $\mathbf{X}'$ and $\mathbf{X}$, and if, for $A_i, B_j \in \mathbf{X}'$, the directed edge from A_i to B_j exists in $\text{SubDAG}_{G'}(\mathbf{X}')$ if and only if the directed edge from A to B exists in $\text{SubDAG}_G(\mathbf{X})$. In such a case we write $\text{SubDAG}_{G'}(\mathbf{X}') \sim \text{SubDAG}_G(\mathbf{X})$. This bijection captures “sameness of the sub-DAGs (both labels and connectivity) up to the identity of the copy-index.”

Next, let us consider subsets of nodes $\mathbf{U}' \subseteq \text{Nodes}(G')$ and $\mathbf{U} \subseteq \text{Nodes}(G)$. Let $\mathbf{X}_{\mathbf{U}'} \subseteq \text{Nodes}(G')$ be the set of nodes comprised of $\mathbf{U}'$ and all ancestors of the nodes of $\mathbf{U}'$ in G' and similarly for $\mathbf{X}_{\mathbf{U}} \subseteq \text{Nodes}(G)$. If $\text{SubDAG}_{G'}(\mathbf{X}_{\mathbf{U}'}) \sim \text{SubDAG}_G(\mathbf{X}_{\mathbf{U}})$ in the sense outlined above, then we write

$$\text{ansubgraph}_{G'}(\mathbf{U}') \sim \text{ansubgraph}_G(\mathbf{U}), \quad (7)$$

where $\text{ansubgraph}_G(\mathbf{U})$ is called the ancestral subgraph of $\mathbf{U}$ in G . In this case, the ancestral subgraph of $\mathbf{U}'$ in G' and that of $\mathbf{U}$ in G are the same up to the identity of the copy-indices.

There are two important notions from the inflation technique that are defined with respect to the correspondence in Eq. (7). The first is the notion of injectable set, defined as follows. If $\mathbf{U}'$ consists entirely of visible nodes of G' , i.e., $\mathbf{U}' \subseteq \text{Vnodes}(G')$, and $\mathbf{U} \subseteq \text{Vnodes}(G)$ is such that $\text{ansubgraph}_{G'}(\mathbf{U}') \sim \text{ansubgraph}_G(\mathbf{U})$, then $\mathbf{U}'$ is called an *injectable set* and $\mathbf{U}$ is the *image of this injectable set* under the dropping of copy indices. The set of injectable sets of G' is denoted $\text{InjectableSets}(G')$ and the set of all their images in G is denoted $\text{ImagesInjectableSets}(G)$.

The second is the very notion of an inflation of a DAG. A DAG G' is an *inflation* of G if and only if, for every $A \in \text{Nodes}(G)$ and $A_i \in \text{Nodes}(G')$ (so that $\text{DropCopyIndex}_{G' \rightarrow G}(A_i) = A$), $\text{ansubgraph}_{G'}(A_i) \sim \text{ansubgraph}_G(A)$. In other words, for G' to be an inflation of G , every *singleton* set of visible nodes in G' must be an injectable set. The set of DAGs that are inflations of G is denoted $\text{Inflations}(G)$.

To explain these concepts further, let us consider an inflation used in the remainder of this work, namely the *AB-Cut inflation* of the triangle scenario, depicted in Fig. 1(b). In this case, the inflated DAG contains just a single copy of each of the visible nodes, A, B, C , and a single copy of two of the latent nodes, namely, L and N , but two copies of the latent node M . The latter are denoted by M_1 and M_2 , while the former are denoted by A_1, B_1, C_1, L_1, N_1 . Consider next the requirement of matching the ancestral subgraphs of visible nodes. The ancestry of each of the visible nodes in the original triangle consists only of the node's parents, so that the ancestral sub-DAG of node A is the v -shaped “collider” DAG with arrows pointing from latent nodes L and M to A (and similarly for B with parents L, N and for C with parents M, N). In the Cut inflation, the situation is the same: the visible node A_1 has ancestry given by the v -shaped DAG with parents L_1 and M_2 , B_1 has parents M_1 and N_1 , and C_1 has parents L_1 and N_1 . By removing the copy-indices (the subscripts) these ancestral sub-DAGs exactly match those of A, B , and C . By the same token, it can be seen that $\{A_1, C_1\}$ is an injectable set: the ancestral subgraph of $\{A_1, C_1\}$ in G' is the w -shaped subgraph made up of A_1, C_1 , their parents L_1, M_2, N_1 and the arrows between them, which corresponds precisely to the subgraph made up of A, B, L, M, N in G . Likewise, $\{B_1, C_1\}$ is also an injectable set.

However, in the *AB-Cut inflation* of the triangle scenario, the set $\{A_1, B_1\}$ is *not* injectable. This can be seen by noting that, in G' , A_1 and B_1 share no common ancestor, whereas A and B *do* share an ancestor in G (i.e., M). While this ancestral independence disallows $\{A_1, B_1\}$ from being an injectable set, it is an example of a related notion, that of an *expressible set*. In the context of this work, namely, when considering DAGs G that have the connectivity of a network, an expressible set of $G' \in \text{Inflations}(G)$ is any set that can be written as the union of injectable sets that share no common ancestors in G' . That is, a subset $\mathbf{Y}' \subseteq \text{Vnodes}(G')$ is an expressible set, i.e., $\mathbf{Y}' \in \text{ExpressibleSets}(G')$, if there exist $\mathbf{U}'_{(1)}, \dots, \mathbf{U}'_{(y)} \in \text{InjectableSets}(G')$ such that $\mathbf{Y}' = \bigcup_{j=1}^y \mathbf{U}'_{(j)}$ and such that for any pair j, k such that $j \neq k$, $\text{ansubgraph}_{G'}(\mathbf{U}'_{(j)}) \cap \text{ansubgraph}_{G'}(\mathbf{U}'_{(k)}) = \emptyset$ [38]. All injectable sets are trivial examples of expressible sets.

Up until this point in our description of the inflation technique, we have not needed to stipulate whether we are considering a classical or quantum causal model (or indeed

a causal model for some other generalized probabilistic theory), a distinction that we refer to as the semantics of the causal model. The semantics specifies the nature of the parameters of the causal model. From this point on, however, what we say is specific to quantum causal models. As noted above, the case of classical causal models can be recovered by restricting attention to density operators that are diagonal relative to some fixed product basis over the subsystems and channels that act as stochastic maps relative to this basis.

We now introduce a map from the *parameters* of a causal model on G , denoted par , to the parameters of a causal model on G' (an inflation of G), denoted par' . In other words, we describe how inflation acts on the parameters of a model. We denote this map from par to par' by $\text{Inflation}_{G \rightarrow G'}$ [39].

The map $\text{Inflation}_{G \rightarrow G'}$ taking a choice of parameters on G to a choice of parameters on $G' \in \text{Inflations}(G)$ is defined by the following conditions: (i) For every visible node A_i in G' , the quantum channel relating A_i to its parents within G' is the same as the quantum channel relating A to its parents within G ,

$$\forall A_i \in \text{Vnodes}(G') : \mathcal{E}_{A_i|\tilde{\text{Pa}}_{G'}(A_i)} = \mathcal{E}_{A|\tilde{\text{Pa}}_G(A)}. \quad (8)$$

(ii) For every latent node L_j in G' , let $\text{Ch}(L_j)$ denote the set of children of L_j in G' and let $\widehat{\text{Ch}}(L_j) := \text{DropCopyIndex}_{G' \rightarrow G}(\text{Ch}(L_j)) \subseteq \text{Ch}(L)$ denote the set of visible nodes of G that are the same up to copy-index as the nodes of $\text{Ch}(L_j)$. The state on L_j is then taken to be the reduced state of the state ρ_L on L in G on the subsystems indexed by the elements of $\widehat{\text{Ch}}(L_j)$. That is,

$$\forall L_j \in \text{Lnodes}(G') : \rho_{L_j} = \text{Tr}_{L(A):A \in \text{Ch}(L) \setminus \widehat{\text{Ch}}(L_j)}[\rho_L], \quad (9)$$

with the understanding that, if $\widehat{\text{Ch}}(L_j) = \text{Ch}(L)$, then $\rho_{L_j} = \rho_L$ [40].

So, why is the inflation map—and the broader machinery of the inflation technique—relevant for problems of causal compatibility? In essence, it allows a question of compatibility with G to be mapped to a question of compatibility with an inflation G' of G . The formal statement of this is given in Proposition 1 below.

Before stating and proving the proposition, let us establish some of the notation to be used throughout the remainder of this section. As above, Y' will continue to denote an expressible set of G' , i.e., $Y' \in \text{ExpressibleSets}(G')$. The set of elements $U'_{(j)} \in \text{InjectableSets}(G')$, for $j = 1, \dots, y$, that are ancestrally independent and make up Y' is denoted $\text{InjectableComponents}(Y')$ (note that $y \in \mathbb{N}$ depends on Y'). The images under the DropCopyIndex map of the $U'_{(j)}$ in $\text{ImagesInjectableSets}(G)$ for a given Y' are denoted $U_{(j)}$, and the set of these is denoted $\text{ImagesInjectableComponents}(Y')$. We have the following:

Proposition 1. Let G' be an inflation of the network G . In this case, if the family of states $\{\rho_U : U \in \text{ImagesInjectableSets}(G)\}$ is compatible with G , then the family of states $\{\sigma_{Y'} : Y' \in \text{ExpressibleSets}(G')\}$, where

$$\sigma_{Y'} := \bigotimes_{U \in \text{ImagesInjectableComponents}(Y')} \rho_U \quad (10)$$

is compatible with G' .

Proof. Suppose that $\{\rho_U : U \in \text{ImagesInjectableSets}(G)\}$ is compatible with G . That means there exists a choice of parameters par on G that realizes a state $\rho_{\text{Vnodes}(G)}$ such that

$$\rho_U = \text{Tr}_{\text{Vnodes}(G) \setminus U}[\rho_{\text{Vnodes}(G)}], \quad (11)$$

for all $U \in \text{ImagesInjectableSets}(G)$. Consider the parameters par' on G' given by $\text{par}' = \text{Inflation}_{G \rightarrow G'}(\text{par})$, which realize some state $\sigma_{\text{Vnodes}(G')}$ on the visible nodes of G' . For any $X' \in \text{InjectableSets}(G')$, with image $X \in \text{ImagesInjectableSets}(G)$, we have that

$$\sigma_{X'} := \text{Tr}_{\text{Vnodes}(G') \setminus X'}[\sigma_{\text{Vnodes}(G')}] \equiv \rho_X. \quad (12)$$

This follows from the definition of injectable set and the definition of the map $\text{Inflation}_{G \rightarrow G'}$.

Suppose $Y' \in \text{ExpressibleSets}(G')$ is such that

$$\begin{aligned} & \text{InjectableComponents}(Y') \\ &= \{U'_{(j)} \in \text{InjectableSets}(G') \mid j = 1, \dots, y\}. \end{aligned} \quad (13)$$

As a consequence of ancestral independence, we get that

$$\sigma_{Y'} := \text{Tr}_{\text{Vnodes}(G') \setminus Y'}[\sigma_{\text{Vnodes}(G')}] \quad (14)$$

$$= \bigotimes_{j=1}^y \text{Tr}_{\text{Vnodes}(G') \setminus U'_{(j)}}[\sigma_{\text{Vnodes}(G')}] \quad (15)$$

$$= \bigotimes_{j=1}^y \sigma_{U'_{(j)}}. \quad (16)$$

Since each $U'_{(j)}$ is injectable, with image $U_{(j)}$, applying Eq. (12) gives that $\sigma_{Y'} = \bigotimes_{j=1}^y \rho_{U_{(j)}}$. As the states $\sigma_{Y'}$ for $Y' \in \text{ExpressibleSets}(G')$ are all marginals of the same state $\sigma_{\text{Vnodes}(G')}$ which is compatible with G' , it is also the case that the family $\{\sigma_{Y'} : Y' \in \text{ExpressibleSets}(G')\}$ is compatible with G' . ■

An example illustrating this proposition for the case where G is the triangle scenario and G' is the AB -Cut inflation is given in Appendix D.

Next, it is useful to define the notion of a causal compatibility inequality.

Let G be a causal structure and let X be a family of subsets of the visible nodes of G . Let I_X denote an inequality that operates on the corresponding family of states, $\{\rho_X : X \in X\}$. Then I_X is a *causal compatibility inequality for the causal structure G* (or a *G -compatibility inequality* for short) whenever it is satisfied by every family of states $\{\rho_X : X \in X\}$ that is compatible with G .

Note that while violation of a causal compatibility inequality for G witnesses the incompatibility of a state with the causal structure G , satisfaction of the inequality does not guarantee compatibility: satisfaction of the inequality merely provides a *necessary* condition for compatibility.

Inflation provides a means of “pulling back” causal compatibility inequalities from the inflation DAG G' to answer questions of causal compatibility with the original DAG G . This is formalized in the following corollary of Proposition 1.

Corollary 1. Let G' be an inflation of a network G and let $\{\rho_U : U \in \text{ImagesInjectableSets}(G)\}$ be a family of states that is compatible with G . Let $T' \subseteq \text{ExpressibleSets}(G')$. If $I_{T'}$ is a causal compatibility inequality for G' operating on families of states $\{\tau_{Y'} : Y' \in T'\}$, then the family of states $\{\sigma_{Y'} : Y' \in T'\}$, defined via

$$\sigma_{Y'} := \bigotimes_{U \in \text{ImagesInjectableComponents}(Y')} \rho_{U_{(j)}}, \quad (17)$$

satisfies $I_{T'}$.

Proof. By Proposition 1, if $\{\rho_U : U \in \text{ImagesInjectableSets}(G)\}$ is compatible with G , then $\{\sigma_{Y'} : Y' \in \text{ExpressibleSets}(G')\}$, with

$$\sigma_{Y'} := \bigotimes_{U \in \text{ImagesInjectableComponents}(Y')} \rho_{U_{(j)}} \quad (18)$$

is compatible with G' . Since the compatibility of $\{\sigma_{Y'} : Y' \in \text{ExpressibleSets}(G')\}$ with G' implies that $\{\sigma_{Y'} : Y' \in T'\}$ is compatible with G' for each $T' \subseteq \text{ExpressibleSets}(G')$, and since $I_{T'}$ is satisfied for all families of states $\{\tau_{Y'} : Y' \in T'\}$ that are compatible with G' , it must also be satisfied for $\{\sigma_{Y'} : Y' \in T'\}$. ■

The utility of this corollary for questions of compatibility with the original causal model G arises from the contrapositive of the above statement: if $I_{T'}$ is *not* satisfied for $\{\sigma_{Y'} : Y' \in T'\}$ with $\sigma_{Y'}$ as in Eq. (17), then $\{\rho_U : U \in \text{ImagesInjectableSets}(G)\}$ cannot be compatible with G . It is in this direction that we must use the above results in the remainder of this work.

It should be noted that all of these results are simply straightforward quantum generalizations of the ones presented in Ref. [15] for the case of classical causal models.

1. The distinction between fanout and nonfanout inflations

An inflation is called *fanout* if it contains a latent node that influences visible nodes that are the same up to copy-indices, that is, if it contains a latent node that influences more than one copy of a visible node from the original DAG. Otherwise, the inflation is termed *nonfanout* [41]. For the triangle scenario, an example of a fanout inflation is the spiral inflation, depicted in Fig. 1(c), while an example of a nonfanout inflation is the Cut inflation, depicted in Fig. 1(b).

If one is considering the causal compatibility problem in quantum causal models, then it is not clear how to make use of a fanout inflation. In particular, the interpretation of a fanned-out latent node cannot be that it is copied and made to influence each of several children that are the same up to copy-indices, because the quantum no-broadcasting theorem prohibits such copying [34]. As such, we here restrict attention to nonfanout inflations when deriving causal compatibility constraints in the case of quantum causal models.

In the case where the visible nodes are classical, so that the compatibility problem concerns a joint probability distribution over the visible nodes, then it is an interesting problem to determine, for a given causal structure, whether there is a difference between what can be realized with classical versus quantum latent nodes. Nonfanout inflations derive constraints on compatible distributions that hold for both types of latent nodes. It is only with fanout inflations that one can derive constraints that can separate the cases of classical and quantum latents. For the Bell scenario, for instance, it is a fanout inflation that allows one to derive Bell inequalities, which are the constraints that establish the existence of a quantum-classical gap in this case.

It is worth noting that some causal structures do not admit of any nontrivial nonfanout inflations. For example, the causal structure known as the bilocality scenario (see, e.g., [42]) is such an example that is moreover a member of the class of causal structures considered here (i.e., it is a network).

B. Example of cut inflation of triangle scenario: Classical case

As noted above, one obtains a description of how inflation can be used to derive causal compatibility inequalities for *classical* causal models by simply restricting to density operators that are diagonal relative to some fixed product basis over the subsystems and channels that act as stochastic maps relative to this basis.

In this article, we will primarily focus on using the inflation technique to derive causal compatibility constraints for the triangle scenario using the cut inflation. We do so first for classical causal models, i.e., using the classical

version of the inflation technique, in order to facilitate a comparison with the case of quantum causal models which is our main focus.

1. Leveraging classical marginal inequalities

We consider the AB -Cut inflation of the triangle scenario, depicted in Fig. 1(b). As noted earlier, the injectable sets of visible nodes in this case are, in addition to all the singleton sets, the two-node sets $\{A_1, C_1\}$ and $\{B_1, C_1\}$. Meanwhile, the two-node set $\{A_1, B_1\}$ is not injectable, but it is expressible. By the classical version of Corollary 1, which follows from taking all density operators to be diagonal in some product basis (see corollary 6 of Ref. [15]), any causal compatibility inequality for the inflation DAG that involves only the expressible sets $\{A_1\}$, $\{B_1\}$, $\{C_1\}$, $\{A_1, B_1\}$, $\{A_1, C_1\}$ and $\{B_1, C_1\}$ defines (by the dropping of copy-indices) a causal compatibility inequality for the original DAG. By considering these sets as marginal contexts, we turn to the question of how to leverage results from the classical marginal problem to derive causal compatibility inequalities on the inflation DAG that are of this type.

We begin by recalling the classical marginal problem on a set of variables $\mathbf{V}$. Any subset of variables is termed a *marginal context*. The set of *all* marginal contexts, which is simply the power set of the set $\mathbf{V}$, we denote by $2^{\mathbf{V}}$. An instance of the classical marginal problem is to determine, for a given set of marginal contexts $S \subseteq 2^{\mathbf{V}}$, and a given set of distributions on each of these contexts, $\{Q_{\mathbf{X}} : \mathbf{X} \in S\}$, whether there is a joint distribution $Q_{\mathbf{V}}$ such that each of the $Q_{\mathbf{X}}$ is recovered as the marginal of $Q_{\mathbf{V}}$ on $\mathbf{X}$, i.e., such that $Q_{\mathbf{X}} = \sum_{\mathbf{V}/\mathbf{X}} Q_{\mathbf{V}}$. In this case, we say that the set of distributions $\{Q_{\mathbf{X}} : \mathbf{X} \in S\}$ satisfies *marginal compatibility*. We are here introducing an important notational convention. When we denote distributions by “ Q ,” such as $\{Q_{\mathbf{X}} : \mathbf{X} \in S\}$, we mean a set of distributions on marginal contexts that may or may not be marginals of a single distribution, whereas if we denote distributions by “ P ,” such as $\{P_{\mathbf{X}} : \mathbf{X} \in S\}$, then they *are* assumed to be marginals of a single distribution.

The most obvious constraint that a set $\{Q_{\mathbf{X}} : \mathbf{X} \in S\}$ must satisfy in order to be marginally compatible is termed the *equimarginal property* and asserts that for any inclusion relation holding among the marginal contexts, i.e., $\mathbf{X}', \mathbf{X} \in S$ such that $\mathbf{X}' \subset \mathbf{X}$, we require $Q_{\mathbf{X}'} := \sum_{\mathbf{X}/\mathbf{X}'} Q_{\mathbf{X}}$. This constraint is straightforward to check, so we will restrict our attention to *nontrivial* constraints. That is, we will only ask about the marginal compatibility of sets $\{Q_{\mathbf{X}} : \mathbf{X} \in S\}$ that satisfy the equimarginal property.

For our example, the set of variables is $\mathbf{V} = \{A, B, C\}$, and the set of marginal contexts of interest is the powerset of $\mathbf{V}$ excluding $\mathbf{V}$ itself, so that $S = 2^{\mathbf{V}} \setminus \mathbf{V} := \{\{A\}, \{B\}, \{C\}, \{AB\}, \{AC\}, \{BC\}\}$. The input to our classical marginal problem in this case is an

equimarginal set of distributions $\{Q_{\mathbf{X}} : \mathbf{X} \in 2^{\mathbf{V}} \setminus \mathbf{V}\} = \{Q_A, Q_B, Q_C, Q_{AB}, Q_{AC}, Q_{BC}\}$.

A necessary condition for such an equimarginal family of distributions to be marginally compatible is that the following inequality be satisfied [21]:

$$\mathbf{1} - Q_A - Q_B - Q_C + Q_{AB} + Q_{AC} + Q_{BC} \geq \mathbf{0}, \quad (19)$$

where the distributions appearing here are conceptualized as functions over the full sample space, $\mathbf{1}$ denotes the function that takes the value 1 everywhere, and $\mathbf{0}$ denotes the function that takes the value 0 everywhere. We refer to this as a *marginal compatibility inequality*.

To emphasize that this is to be conceptualized as an inequality on a family of distributions $\{Q_{\mathbf{X}} : \mathbf{X} \in 2^{\mathbf{V}} \setminus \mathbf{V}\}$, It is useful to write it as

$$\Delta(\{Q_{\mathbf{X}} : \mathbf{X} \in 2^{\mathbf{V}} \setminus \mathbf{V}\}) \geq \mathbf{0}. \quad (20)$$

where $\Delta(\{Q_{\mathbf{X}} : \mathbf{X} \in 2^{\mathbf{V}} \setminus \mathbf{V}\}) := \mathbf{1} - Q_A - Q_B - Q_C + Q_{AB} + Q_{AC} + Q_{BC}$.

Also, if one evaluates this functional inequality at $A = a, B = b, C = c$ for each set of values a, b, c , one obtains a set of inequalities on the real parameters appearing in these distributions, specifically,

$$\forall a, b, c : 1 - Q_A(a) - Q_B(b) - Q_C(c) + Q_{AB}(ab) + Q_{AC}(ac) + Q_{BC}(bc) \geq 0. \quad (21)$$

If the constraint is presented in this form, then we have a set of inequalities, rather than a single inequality. In this case, we term them *marginal compatibility inequalities* (plural).

Now consider a distribution $P_{A_1 B_1 C_1}$ on the variables appearing in the AB -Cut inflation DAG, namely, A_1, B_1 and C_1 . The marginal compatibility inequality above implies that

$$\mathbf{1} - P_{A_1} - P_{B_1} - P_{C_1} + P_{A_1 B_1} + P_{A_1 C_1} + P_{B_1 C_1} \geq \mathbf{0}. \quad (22)$$

Note that this constraint follows simply from classical probability theory and has nothing to do with the causal structure of the AB -Cut inflation DAG. However, we will now combine it with a constraint that *does* follow from this causal structure.

Specifically, we consider the d -separation relations among the visible nodes. In brief, the d -separation relations in a given DAG G are the graphical description of the conditional independence of variables (or sets thereof) associated with the nodes of G for any distribution compatible with G . These descriptions are given in terms of paths between the nodes in question (see, e.g., Refs. [1, 12] for a formal definition of d -separation). In the case of the AB -Cut inflation, there is one such relation, namely, that A_1 and

B_1 are d -separated given the empty set. This holds because the only path between A_1 and B_1 in the AB -Cut inflation passes through C_1 , which is a collider—see Refs. [1, 12]. As a consequence, the variables A_1 and B_1 are marginally independent (which is equivalent to independence conditioned on the empty set) in any distribution compatible with the AB -Cut inflation. That is, for any such distribution $P_{A_1 B_1 C_1}$, we require

$$P_{A_1 B_1} = P_{A_1} P_{B_1}. \quad (23)$$

To get a nontrivial causal compatibility inequality on the marginals of $P_{A_1 B_1 C_1}$, it suffices to combine the equality constraint of Eq. (23) with the marginal compatibility inequality of Eq. (19) to obtain

$$1 - P_{A_1} - P_{B_1} - P_{C_1} + P_{A_1} P_{B_1} + P_{A_1 C_1} + P_{B_1 C_1} \geq 0. \quad (24)$$

[Note the difference to Eq. (22), namely, that $P_{A_1} P_{B_1}$ appears in place of $P_{A_1 B_1}$.]

From this, we can infer a causal compatibility inequality for the triangle scenario DAG. It suffices to note that the inequality of Eq. (24) is a polynomial function of $P_{A_1}, P_{B_1}, P_{C_1}, P_{A_1 C_1}$ and $P_{B_1 C_1}$ and that these are all marginals on *injectable sets* of visible nodes in the inflation DAG. By Corollary 1, we infer that the inequality having the same functional form as Eq. (24) but where A_1, B_1 and C_1 are replaced by A, B , and C respectively, namely,

$$1 - P_A - P_B - P_C + P_A P_B + P_{AC} + P_{BC} \geq 0, \quad (25)$$

is a causal compatibility inequality for the triangle scenario in terms of the marginals P_A, P_B, P_C, P_{AC} , and P_{BC} of P_{ABC} . If a given joint distribution P_{ABC} violates the inequality of Eq. (25), then it is incompatible with the triangle scenario. Following the terminology of a “ G -compatibility inequality” introduced above, it is appropriate to refer to such an inequality on P_{ABC} as a *triangle-compatibility inequality*.

One can of course consider Cut Inflations where the Cut is between B and C or between A and C , rather than being between A and B . We get analogous inequalities for each case, namely, for each $x, y, z \in \{A, B, C\}$ such that $x \neq y \neq z$,

$$1 - P_x - P_y - P_z + P_x P_y + P_{xz} + P_{yz} \geq 0. \quad (26)$$

A violation of any of these inequalities suffices to demonstrate triangle-incompatibility. In general, it will be clear from the context and the notation which inequality is being used [such as via the use of subscripts as in, e.g., Eq. (27) below].

Because the inequality of Eq. (26) expresses a necessary condition on the joint distribution P_{ABC} for triangle-compatibility using the xy -Cut inflation, it is useful to write

it as

$$I_{xy}(P_{ABC}) \geq 0, \quad (27)$$

where

$$I_{xy}(P_{ABC}) := 1 - P_x - P_y - P_z + P_x P_y + P_{xz} + P_{yz},$$

and where P_x is the marginal on the singleton set x , P_{xz} is the marginal on the two-variable set xz , etcetera.

2. Some distributions whose triangle-incompatibility is witnessed

We now explore some of the conclusions that can be inferred from this triangle-compatibility inequality.

As a simple example, consider the following tripartite distribution, which we will refer to as the *GHZ distribution* [because of its similarity with the Greenberger-Horne-Zeilinger (GHZ) state in quantum theory [43]],

$$P_{ABC}^{(\text{GHZ})} = \frac{1}{2} ([000]_{ABC} + [111]_{ABC}), \quad (28)$$

where $[abc]_{ABC}$ denotes the point distribution wherein all the probabilistic weight is on $A = a, B = b$, and $C = c$ [44]. It is straightforward to see that $P_{ABC}^{(\text{GHZ})}$ violates a triangle-compatibility inequality. For example, using Eq. (25) and taking $A = 0, B = 0, C = 1$, we find that the left-hand-side evaluates to $1 - \frac{1}{2} - \frac{1}{2} - \frac{1}{2} + \frac{1}{4} + 0 + 0 = -\frac{1}{4}$. Since this is negative, the inequality is violated. It follows that the GHZ distribution is incompatible with the triangle scenario.

It is worth recalling that violations of a G -compatibility inequality by a distribution witnesses the incompatibility of that distribution with the causal structure G , but satisfaction of such inequalities by a distribution does not guarantee that it is compatible. A good example of this is the following distribution:

$$P_{ABC}^{(\text{W})} = \frac{1}{3} ([100]_{ABC} + [010]_{ABC} + [001]_{ABC}), \quad (29)$$

which is termed the “W distribution” (this distribution is likewise inspired by a quantum state, namely, the W-state of Ref. [45]). $P_{ABC}^{(\text{W})}$ can easily be verified to *satisfy* the triangle-compatibility inequalities (satisfaction of the inequality for any of the Cuts implies satisfaction of the inequalities for the other Cuts due to the symmetries in the distribution), but it is nonetheless incompatible with the triangle scenario. Triangle-incompatibility of the W distribution is established in Ref. [15] using the Spiral inflation of the triangle scenario, which is depicted in Fig. 1(c) [46].

C. Example of cut inflation of triangle scenario: Quantum case

Again, we consider the AB -Cut inflation of the triangle scenario, depicted in Fig. 1(b). Analogously to the classical case, Corollary 1 guarantees that if we can identify a causal compatibility inequality on the inflation DAG that involves only the expressible sets $\{A_1\}$, $\{B_1\}$, $\{C_1\}$, $\{A_1, B_1\}$, $\{A_1, C_1\}$ and $\{B_1, C_1\}$, then dropping the copy-indices yields a causal compatibility inequality for the triangle scenario. We find such a causal compatibility inequality on the inflation DAG by leveraging the results from the quantum marginal problem. This is the sense in which the fully quantum inflation technique allows questions of causal compatibility to be related to quantum marginal problems, allowing progress on the latter to be brought to bear on the former.

1. Leveraging quantum marginal inequalities

This subsection presents a family of operator inequalities describing solutions to a particular instance of the quantum marginal problem and demonstrates how these can be leveraged in fully quantum inflation. Specifically, the extra constraints enforced by the causal structure of the inflation DAG (such as factorization constraints) can be substituted into these operator inequalities to yield modified operator inequalities that constitute causal compatibility inequalities for the inflation DAG.

The quantum version of the marginal problem is defined precisely as the classical version, but where we consider joint quantum states rather than joint probability distributions, and marginalization corresponds to the partial trace operation. Consequently, if $\mathbf{V}$ denotes the full set of quantum systems under consideration, an instance of the quantum marginal problem is to determine, for a given set of marginal contexts $S \subseteq 2^{\mathbf{V}}$, and a given set of quantum states on each of these contexts, $\{\sigma_{\mathbf{X}} : \mathbf{X} \in S\}$, whether there is a joint quantum state $\sigma_{\mathbf{V}}$ such that each of the $\sigma_{\mathbf{X}}$ is recovered as the marginal of $\sigma_{\mathbf{V}}$ on $\mathbf{X}$, i.e., such that $\sigma_{\mathbf{X}} = \text{Tr}_{\mathbf{V} \setminus \mathbf{X}}[\sigma_{\mathbf{V}}]$. In this case, we say that the set of states $\{\sigma_{\mathbf{X}} : \mathbf{X} \in S\}$ satisfy marginal compatibility. The notations σ and ρ will parallel those of Q and P in the classical case: $\{\sigma_{\mathbf{X}} : \mathbf{X} \in S\}$ denotes a set of states on marginal contexts that may or may not be marginals of a single joint state, whereas if we write $\{\rho_{\mathbf{X}} : \mathbf{X} \in S\}$, then they are assumed to be marginals of a single joint state.

In Ref. [19], Hall introduced a necessary condition that the marginals of any quantum state on a (finite-dimensional) composite Hilbert space consisting of an odd number of subsystems must satisfy (c.f. [19, Thm 1] and the discussion thereafter). Suppose $\mathbf{V}$ denotes a set of quantum systems and let $\sigma_{\mathbf{X}} \in \mathcal{L}(\bigotimes_{X \in \mathbf{X}} \mathcal{H}_X)$ denote a joint quantum state on $\mathbf{X} \subseteq \mathbf{V}$ (i.e., a positive semidefinite operator with unit trace). The necessary condition on a set $\{\sigma_{\mathbf{X}} : \mathbf{X} \in 2^{\mathbf{V}} \setminus \mathbf{V}\}$ of states to be the marginals of a

single state $\sigma_{\mathbf{V}}$ when the set $\mathbf{V}$ is of odd cardinality is the following operator inequality:

$$\Delta(\{\sigma_{\mathbf{X}} : \mathbf{X} \in 2^{\mathbf{V}} \setminus \mathbf{V}\}) \geq 0, \quad (30)$$

where

$$\Delta(\{\sigma_{\mathbf{X}} : \mathbf{X} \in 2^{\mathbf{V}} \setminus \mathbf{V}\}) := \sum_{\mathbf{X} \in 2^{\mathbf{V}} \setminus \mathbf{V}} (-1)^{|\mathbf{X}|} \sigma_{\mathbf{X}} \otimes \mathbb{1}_{\mathbf{V} \setminus \mathbf{X}}, \quad (31)$$

with $|\mathbf{X}|$ denoting the cardinality of the set $\mathbf{X}$, with $\mathbb{1}_{\mathbf{V} \setminus \mathbf{X}}$ denoting the identity operator on the subsystems in $\mathbf{V} \setminus \mathbf{X}$, and with $\geq$ denoting the standard partial order relation over Hermitian operators (i.e., $M \geq N$ if and only if $M - N$ is a positive semidefinite operator), so that an operator inequality of the form $O \geq 0$ signifies that O is positive semidefinite [47].

In this work, we focus on the case of $\mathbf{V} = \{A, B, C\}$, and thus on the operator

$$\begin{aligned} \Delta(\{\sigma_{\mathbf{X}} : \mathbf{X} \in 2^{\mathbf{V}} \setminus \mathbf{V}\}) &= \mathbb{1}_{ABC} - \sigma_A \otimes \mathbb{1}_{BC} - \sigma_B \otimes \mathbb{1}_{AC} - \sigma_C \otimes \mathbb{1}_{AB} \\ &\quad + \sigma_{AB} \otimes \mathbb{1}_C + \sigma_{AC} \otimes \mathbb{1}_B + \sigma_{BC} \otimes \mathbb{1}_A. \end{aligned} \quad (35)$$

It is convenient to suppress tensor products with identity operators, as well as the subscripts on the remaining identity operator on the entire space, and simply write

$$\begin{aligned} \Delta(\{\sigma_{\mathbf{X}} : \mathbf{X} \in 2^{\mathbf{V}} \setminus \mathbf{V}\}) &= \mathbb{1} - \sigma_A - \sigma_B - \sigma_C + \sigma_{AB} + \sigma_{AC} + \sigma_{BC}. \end{aligned} \quad (36)$$

Because $\mathbf{V}$ is of odd cardinality, we infer from Hall's result that $\Delta(\{\sigma_{\mathbf{X}} : \mathbf{X} \in 2^{\mathbf{V}} \setminus \mathbf{V}\})$ must be positive semidefinite when the elements of $\{\sigma_{\mathbf{X}} : \mathbf{X} \in 2^{\mathbf{V}} \setminus \mathbf{V}\}$ are marginals of a single state $\sigma_{\mathbf{V}}$, so that

$$\mathbb{1} - \sigma_A - \sigma_B - \sigma_C + \sigma_{AB} + \sigma_{AC} + \sigma_{BC} \geq 0. \quad (37)$$

In this form, the operator inequality is clearly the quantum counterpart of Eq. (19). We refer to it as a *quantum marginal compatibility inequality*.

Now consider a state $\rho_{A_1 B_1 C_1}$ on the systems that appear in the AB -Cut inflation DAG, namely, A_1 , B_1 and C_1 . The quantum marginal compatibility inequality above implies that

$$\mathbb{1} - \rho_{A_1} - \rho_{B_1} - \rho_{C_1} + \rho_{A_1 B_1} + \rho_{A_1 C_1} + \rho_{B_1 C_1} \geq 0. \quad (38)$$

As with the constraint of Eq. (22) in the classical case, this constraint has nothing to do with the causal structure of the AB -Cut inflation DAG, but we can combine it with such a constraint to obtain a causal compatibility inequality.

Again, we leverage the fact that, in the AB -Cut inflation DAG, A_1 and B_1 are d -separated given the empty set. It follows that any state $\rho_{A_1 B_1 C_1}$ that is compatible with this DAG must satisfy

$$\rho_{A_1 B_1} = \rho_{A_1} \otimes \rho_{B_1}. \quad (39)$$

To get a nontrivial causal compatibility inequality for the AB -Cut inflation DAG, we combine the equality constraint of Eq. (39) with the quantum marginal compatibility inequality of Eq. (38) to obtain

$$\mathbb{1} - \rho_{A_1} - \rho_{B_1} - \rho_{C_1} + \rho_{A_1} \otimes \rho_{B_1} + \rho_{A_1 C_1} + \rho_{B_1 C_1} \geq 0. \quad (40)$$

Finally, we can use this together with Corollary 1 to obtain a causal compatibility inequality for the original triangle scenario DAG. Because the inequality is a polynomial function of $\rho_{A_1}, \rho_{B_1}, \rho_{C_1}, \rho_{A_1 C_1}$ and $\rho_{B_1 C_1}$ and because these are all marginals on *injectable sets* of visible nodes in the inflation DAG, the inequality having the same functional form as Eq. (24) but where A_1, B_1 and C_1 are replaced by A, B , and C respectively,

$$\mathbb{1} - \rho_A - \rho_B - \rho_C + \rho_A \otimes \rho_B + \rho_{AC} + \rho_{BC} \geq 0 \quad (41)$$

is a causal compatibility inequality for the triangle scenario.

We refer to this operator inequality as a triangle-compatibility inequality for the quantum state ρ_{ABC} . It is convenient to write this as

$$I_{AB}(\rho_{ABC}) \geq 0, \quad (42)$$

where

$$I_{AB}(\rho_{ABC}) := \mathbb{1} - \rho_A - \rho_B - \rho_C + \rho_A \otimes \rho_B + \rho_{AC} + \rho_{BC}. \quad (43)$$

Summarizing, if the state ρ_{ABC} is triangle-compatible, then $I_{AB}(\rho_{ABC})$ is a positive operator. Conversely, if $I_{AB}(\rho_{ABC})$ is found to be nonpositive, then ρ_{ABC} is triangle-incompatible. Note that $I_{AB}(\rho_{ABC})$ can be a positive operator even though ρ_{ABC} is triangle-incompatible, which is why the nonpositivity of $I_{AB}(\rho_{ABC})$ is only a necessary and not a sufficient condition for triangle-incompatibility. We refer to the operator $I_{AB}(\rho_{ABC})$ as a triangle-incompatibility witness.

As we will also be considering Cut inflations between the visible nodes A and C and between B and C , it is convenient to define, for a given ρ_{ABC} ,

$$I_{xy}(\rho_{ABC}) = \mathbb{1} - \rho_x - \rho_y - \rho_z + \rho_x \otimes \rho_y + \rho_{xz} + \rho_{yz}, \quad (44)$$

where $x, y, z \in \{A, B, C\}$ such that $x \neq y \neq z$ and where we are suppressing tensor products with identity operators. For each type of cut, we have a corresponding triangle-incompatibility inequality, $I_{xy}(\rho_{ABC}) \geq 0$.

It is worth noting that $I_{xy}(\rho_{ABC})$ can be equivalently expressed as

$$I_{xy}(\rho_{ABC}) = \Delta(\{\rho_{\mathbf{X}} : \mathbf{X} \in 2^{\mathbf{V}} \setminus \mathbf{V}\}) + \rho_x \otimes \rho_y - \rho_{xy}. \quad (45)$$

2. Some technical results

Before proceeding to our general results, we note a few useful facts about the operators $I_{xy}(\rho_{ABC})$. Since $\Delta(\{\rho_{\mathbf{X}} : \mathbf{X} \in 2^{\mathbf{V}} \setminus \mathbf{V}\})$ is guaranteed to be positive, the only chance for demonstrating that $I_{xy}(\rho_{ABC})$ is nonpositive must derive from the nonpositivity of $\rho_x \otimes \rho_y - \rho_{xy}$. We note the following:

Lemma 1. If $\rho_{xy} \neq \rho_x \otimes \rho_y$ then $\rho_x \otimes \rho_y - \rho_{xy} \not\geq 0$.

The proof is given in Appendix A 1. Considered as an operator on $\mathcal{H}_x \otimes \mathcal{H}_y$, let us write

$$\rho_x \otimes \rho_y - \rho_{xy} = v_{xy}^+ - v_{xy}^-, \quad (46)$$

where the $\{v_{xy}^\pm\}_{xy \in \{AB, AC, BC\}}$ are positive semidefinite and where v_{xy}^+ is mutually orthogonal to v_{xy}^- relative to the Hilbert-Schmidt inner product. The above lemma guarantees that v_{xy}^- is nonzero and also positive semidefinite whenever $\rho_{xy} \neq \rho_x \otimes \rho_y$. Clearly, if ρ_{ABC} is such that there exists some $|\Phi\rangle \in \text{supp}(v_{xy}^- \otimes \mathbb{1}_z) \cap \ker(\Delta(\{\rho_{\mathbf{X}} : \mathbf{X} \in 2^{\mathbf{V}} \setminus \mathbf{V}\}))$ for some $x, y, z \in \{A, B, C\}$ such that $x \neq y \neq z$ then

$$\langle \Phi | I_{xy}(\rho_{ABC}) | \Phi \rangle < 0, \quad (47)$$

demonstrating that ρ_{ABC} is triangle-incompatible. Despite the fact that the existence of such a $|\Phi\rangle$ is not *a priori* necessary for demonstrating the triangle-incompatibility of ρ_{ABC} , it is sufficient, so this constitutes a fruitful method for deriving such results, as we will see further on. We state it as a proposition for later reference:

Proposition 2. Let ρ_{ABC} be a quantum state on the set of visible nodes $\mathbf{V} = \{A, B, C\}$, and let $\Delta(\{\rho_{\mathbf{X}} : \mathbf{X} \in 2^{\mathbf{V}} \setminus \mathbf{V}\})$ and v_{xy}^- be defined in terms of it via Eqs. (36) and (46). If

$$\text{supp}(v_{xy}^- \otimes \mathbb{1}_z) \cap \ker(\Delta(\{\rho_{\mathbf{X}} : \mathbf{X} \in 2^{\mathbf{V}} \setminus \mathbf{V}\})) \neq \emptyset, \quad (48)$$

for some $x, y, z \in \{A, B, C\}$ such that $x \neq y \neq z$, then ρ_{ABC} is triangle-incompatible.

One further advantage of evaluating compatibility with the triangle scenario by evaluating whether the operator $I_{xy}(\rho_{ABC})$ is positive semidefinite consists in the finer-grained understanding of *how* incompatibility of a given state can be shown in certain cases. If there exists a pure product state $|\Phi\rangle = |\phi\rangle_A |\phi'\rangle_B |\phi''\rangle_C$ such that $\langle \Phi | I_{xy}(\rho_{ABC}) | \Phi \rangle < 0$, then it is possible to get a verdict of triangle-incompatibility for ρ_{ABC} purely by local

measurement statistics, i.e., by measuring locally on A according to the basis determined by $|\phi\rangle_A$, and similarly for B and C . We will see shortly why the question of whether one can witness incompatibility using the distribution obtained from local measurements is significant.

3. Some states whose triangle-incompatibility is witnessed

We begin by considering quantum states ρ_{ABC} that simply encode a classical distribution. Any quantum state that is diagonal in the computation basis, for instance, merely encodes a classical distribution over binary variables. The quantum state encoding the GHZ distribution is

$$\begin{aligned}\rho^{(\text{GHZdistn})} &= \frac{1}{2} (|000\rangle\langle 000|_{ABC} + |111\rangle\langle 111|_{ABC}) \\ &:= \sum_{a,b,c} P^{(\text{GHZ})}(a,b,c) |abc\rangle\langle abc|_{ABC},\end{aligned}\quad (49)$$

while the one encoding the W distribution is

$$\begin{aligned}\rho^{(\text{Wdistn})} &:= \frac{1}{3} (|100\rangle\langle 100|_{ABC} + |010\rangle\langle 010|_{ABC} \\ &\quad + |001\rangle\langle 001|_{ABC}) \\ &= \sum_{a,b,c} P^{(\text{W})}(a,b,c) |abc\rangle\langle abc|_{ABC}.\end{aligned}\quad (50)$$

Note that asking about the triangle-compatibility of a state that encodes a distribution in a quantum causal model is not equivalent to asking about the triangle-compatibility of the corresponding distribution in a classical causal model. This is because in the first case, one allows the latent nodes to be quantum while in the second case they are constrained to be classical, and it can happen that a given distribution is realizable in the first but not the second type of model. Indeed, for the case of the triangle scenario, the existence of a gap in the sorts of distributions that are realizable using quantum latent nodes versus those that are realizable using classical latent nodes was shown in Ref. [5] and further studied in Refs. [48,49].

To settle questions about G -compatibility of a state that encodes a distribution, it suffices to use a version of the inflation technique that tests for the G -compatibility of a distribution on the visible nodes when the latent nodes are allowed to be quantum. The standard inflation technique provides the means of doing so: as long as one considers a nonfanout inflation, the technique can witness G -incompatibility of a distribution even if the latent nodes are quantum [15]. One can also consider latent nodes that are quantum using fanout inflations by making use of the quantum inflation technique introduced in Ref. [31]. The point is that fully quantum inflation is not required for states that encode a distribution.

In the case of the GHZ distribution, its triangle-incompatibility was established in Ref. [15] using

the standard inflation technique with the Cut inflation. Given that the latter is nonfanout, its incompatibility holds even for quantum latent nodes.

As noted previously, the triangle-incompatibility of the W distribution can also be established using a nonfanout inflation, namely, the Ring inflation (see the discussion in Ref. [46]), so the triangle-incompatibility of the W distribution also holds even for quantum latent nodes.

Whether fully quantum inflation might provide a *more efficient means* of witnessing triangle-incompatibility for such states remains a question for future research. In any case, we move on now to consider quantum states that are not merely encoding probability distributions.

Consider the GHZ state

$$|\text{GHZ}\rangle := \frac{1}{\sqrt{2}} (|000\rangle_{ABC} + |111\rangle_{ABC}) \quad (51)$$

and the W state,

$$|\text{W}\rangle := \frac{1}{\sqrt{3}} (|100\rangle_{ABC} + |010\rangle_{ABC} + |001\rangle_{ABC}), \quad (52)$$

which differ from the states in Eqs. (49) and (50) by being coherent superpositions of the relevant states rather than incoherent mixtures. Both of these are found to still violate the triangle-compatibility inequality obtained from fully quantum inflation, i.e., Eq. (41), and so both are triangle-incompatible. This can be verified by direct computation (or inferred from Theorem 1).

We again pause to ask whether fully quantum inflation was *necessary* to reach the conclusion of triangle-incompatibility for these states.

In fact, fully quantum inflation is *not* needed to see that the GHZ state is triangle-incompatible. It suffices to note that if one implements local measurements in the computation basis on the GHZ state, one prepares the GHZ distribution, or, equivalently, the quantum state that encodes the GHZ distribution, Eq. (49). Such local measurements are consistent with the causal structure of the triangle scenario, so the possibility of transforming the GHZ state into the state encoding the GHZ distribution in this way means that if the GHZ state is realizable in a quantum causal model within the triangle scenario then so is the state encoding the GHZ distribution. The contrapositive of this statement is that if the state encoding the GHZ distribution is triangle-incompatible then so is the GHZ state. But we established earlier in this section that the state encoding the GHZ distribution is indeed triangle-incompatible. Note, moreover, that the triangle-incompatibility of the state encoding the GHZ distribution can be established with the Cut inflation.

In the case of the W state, fully quantum inflation is also not needed to establish triangle-incompatibility. Again, we can implement local measurements in the computation basis to convert the W state into the state encoding

the W distribution and then make use of the fact that the state encoding the W distribution is shown to be triangle-incompatible using the standard inflation technique with a nonfanout inflation, as noted above.

Unlike the situation with the GHZ distribution, the conclusion of triangle-incompatibility for the W distribution cannot be obtained using the Cut inflation DAG; one must instead use a nonfanout inflation that lies higher in the hierarchy of inflations [50], termed the Ring inflation. Nonetheless, the question remains of whether some *other* choice of local measurement on the W state might lead to a distribution whose triangle-incompatibility is witnessable by the Cut inflation [51]. This does indeed turn out to be the case! By locally measuring each subsystem of the W state in the Pauli- X basis, a probability distribution is produced that can be demonstrated to be triangle-incompatible using the AB -Cut inflation (some details of this calculation are presented in Appendix A 2).

Generalizing beyond the triangle scenario example, two questions arise regarding whether a conclusion of G -incompatibility for some quantum state could have been reached without requiring the “big guns” of fully quantum inflation. The first question is whether it could have been reached just using the standard inflation technique for some nonfanout inflation DAG [15] or using the quantum inflation technique for some fanout inflation DAG [31]. The second question is whether this same conclusion could have been reached using the standard inflation technique with the very same inflation DAG that was used to establish the conclusion using the fully quantum inflation technique. More precisely, the second question is: if the G -incompatibility of a *state* can be witnessed by an inflation G' , is there always some choice of local measurements yielding a distribution whose G -incompatibility can also be witnessed by G' ?

When one can prove incompatibility of a state by leveraging the incompatibility of a distribution obtained from this state by local measurements, we will say that the state incompatibility is *distribution-witnessable*. We will also say that the proof of incompatibility of a state has *piggybacked* on a proof of incompatibility of a distribution.

Using this terminology, the first question is whether there are examples of G -incompatibility results for states that are not distribution-witnessable, and the second question is whether there are examples of G -incompatibility results for states that are not distribution-witnessable *using the same inflation DAG*.

At issue here is whether a test of state incompatibility leveraging the quantum marginal problem, i.e., the fully quantum inflation technique, is strictly more powerful than a test based on results about the classical marginal problem.

In this article, we will focus on the second question. In Sec. IV B, we will show that it receives a negative answer: there are instances of G -incompatibility results for

states that are not distribution-witnessable using the same inflation DAG.

We do not settle the first question here. Consequently, it might be the case that any given G -incompatibility result for a state obtained using an inflation DAG G' can always be inferred from the G -incompatibility of a distribution obtained from the state by some local measurements, by using a different inflation DAG G'' that is at a higher level than G' in the inflation hierarchy of Ref. [50]. It is worth noting, however, that even if this is the case, the utility of this sort of piggybacking technique is limited. First, one requires an algorithm for determining the correct choice of local measurements. Second, the computational cost of a compatibility test increases significantly as one moves up the inflation hierarchy of Ref. [50]. Both facts imply that there is a computational advantage to testing state compatibility directly using fully quantum inflation.

IV. QUBIT VISIBLE NODES

In this section, we begin to showcase the utility of these new ways of witnessing the incompatibility of a quantum state with a given causal structure. We consider the triangle scenario where each of the visible nodes corresponds to a qubit and we investigate the compatibility of both pure (Sec. IV A) and mixed (Sec. IV C) three-qubit states. In Sec. IV B, we consider the question of which states have distribution-witnessable incompatibility for a given inflation DAG and show that there are examples of incompatibility that are not distribution-witnessable.

A. The quantum compatibility problem for pure-states

It is straightforward to see that any tripartite pure-state that factorizes (i.e., is a product state) across some bipartition ($A|BC$, $B|AC$, or $C|AB$) is compatible with the triangle scenario. For example, suppose that ρ_{ABC} is the state $|\phi\rangle\langle\phi|_{AB} \otimes |\phi'\rangle\langle\phi'|_C$ for some $|\phi\rangle_{AB}$ and $|\phi'\rangle_C$. It suffices to illustrate parameters for the causal model such that the condition of Eq. (4) can be satisfied: (i) let $\mathcal{H}_{M^{(B)}} \cong \mathcal{H}_B$, $\mathcal{H}_{M^{(A)}} \cong \mathcal{H}_A$, and $\mathcal{H}_{N^{(C)}} \cong \mathcal{H}_C$, where $\cong$ denotes the existence of an isometry, let $\mathcal{H}_{N^{(B)}}$ and $\mathcal{H}_L$ be arbitrary (for example, they could be one dimensional), and take $\varrho_{M^{(A)}M^{(B)}} = |\phi\rangle\langle\phi|_{M^{(A)}M^{(B)}}$, $\varrho_{N^{(B)}N^{(C)}} = \varrho_{N^{(B)}} \otimes |\phi'\rangle\langle\phi'|_{N^{(C)}}$ with $\varrho_{N^{(B)}}$ arbitrary, and ϱ_L similarly arbitrary; (ii) take $\mathcal{E}_{A|L^{(A)}M^{(A)}} = \text{Tr}_{L^{(A)}} \otimes \mathcal{I}_{A|M^{(A)}}$, i.e., an identity channel from $\mathcal{H}_{M^{(A)}}$ to $\mathcal{H}_A$ and a trace over $\mathcal{H}_{L^{(A)}}$, $\mathcal{E}_{B|M^{(B)}N^{(B)}} = \mathcal{I}_{B|M^{(B)}} \otimes \text{Tr}_{N^{(B)}}$, i.e., an identity channel from $\mathcal{H}_{M^{(B)}}$ to $\mathcal{H}_B$ and a trace over $\mathcal{H}_{N^{(B)}}$, and $\mathcal{E}_{C|L^{(C)}N^{(C)}} = \text{Tr}_{L^{(C)}} \otimes \mathcal{I}_{C|N^{(C)}}$, i.e., an identity channel from $\mathcal{H}_{N^{(C)}}$ to $\mathcal{H}_C$ and a trace over $\mathcal{H}_{L^{(C)}}$.

Furthermore, among three-qubit pure-states, those that factorize across a bipartition (i.e., the biseparable ones) are the *only* states that are triangle-compatible. In other words, in the case of three-qubit pure-states, the boundary between triangle-compatible and triangle-incompatible

coincides precisely with the boundary between those that factorize across a bipartition and those that do not.

Theorem 1. For A , B , and C qubits and a joint quantum state that is pure, $\rho_{ABC} = |\psi\rangle\langle\psi|_{ABC}$, the state is triangle-compatible if and only if it is factorizing across a bipartition (i.e., it is a biseparable pure-state).

The proof of the “if” half is given above. The proof of the “only if” half, which is given in Appendix A 3, consists in applying Lemma 1 to each of the marginals of ρ_{ABC} and finding that the sufficient condition of Proposition 2, namely Eq. (48), holds, from which the result follows.

As noted in the Introduction, Ref. [26] also considered the problem of compatibility of tripartite states with the triangle scenario, but restricting attention to local unitaries (from subsystems of the latent nodes to the visible nodes) rather than arbitrary local channels. In other words, as noted in the Introduction, Ref. [26] studied the set of LUSR2WSE-preparable states. For the purpose of preparing *pure* tripartite states, the shared randomness is irrelevant, so that the free operations used in Ref. [26] and in the above theorem are LU2WSE and LO2WSE respectively. It is possible that in the case of preparing *pure* tripartite states, arbitrary quantum channels offer no additional power relative to unitary channels. If a proof of this latter claim were found, then our Theorem 1 could be obtained as a corollary of Observation 5 from Ref. [26]. Unfortunately, we have not been able to settle this question one way or the other. In any event, the proof technique used here to establish Theorem 1 is quite different from that used to establish Observation 5 in Ref. [26].

B. Examples of incompatibility that are not distribution-witnessable

In Sec. III C 3, we noted that in assessing incompatibility of a quantum state with a given network via some inflation, it is not necessarily the case that this conclusion could be reached by first converting the state into a distribution through local measurements and then witnessing the incompatibility of this distribution using the same inflation DAG. We now prove this result, which we formalize by the following proposition:

Proposition 3. There exist states that are G -incompatible, but for which this incompatibility is not distribution-witnessable with respect to the same inflation of G .

Certain details of the proof are given in Appendix A 4, but the main thrust is given here. The proof considers the family of pure-states $\rho_{ABC}(t) = |\Psi(t)\rangle\langle\Psi(t)|$ where

$$|\Psi(t)\rangle = \frac{\sqrt{t-2}}{\sqrt{t}} |100\rangle + \frac{1}{\sqrt{t}} |001\rangle + \frac{1}{\sqrt{t}} |010\rangle, \quad (53)$$

with t being a real parameter in the interval $[3, \infty)$. We demonstrate that the triangle-incompatibility witness $I_{AB}(\rho_{ABC}(t))$ is not positive for all t under consideration, meaning that every $\rho_{ABC}(t)$ is triangle-incompatible. To give a concrete example: taking t_* such that $((\sqrt{t_*}-2)/\sqrt{t_*}) = 0.9$ (so that the amplitude of each of the other two terms is $(1/\sqrt{t_*}) = \sqrt{0.095}$), we have that

$$I_{AB}(\rho_{ABC}(t_*)) = \begin{bmatrix} 0.733\,05 & 0 & 0 & 0 & 0 & 0.277\,399 & 0 & 0 \\ 0 & 0.018\,05 & 0.095 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0.095 & 0.171\,95 & 0 & 0 & 0 & 0 & 0.277\,399 \\ 0 & 0 & 0 & 0.076\,95 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.076\,95 & 0 & 0 & 0 \\ 0.277\,399 & 0 & 0 & 0 & 0 & 0.171\,95 & 0.095 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.095 & 0.018\,05 & 0 \\ 0 & 0 & 0.277\,399 & 0 & 0 & 0 & 0 & 0.733\,05 \end{bmatrix}, \quad (54)$$

which has a negative eigenvalue $-0.052\,988\,9$ of multiplicity 2.

To demonstrate that there exist values for t such that the triangle-incompatibility of $\rho_{ABC}(t)$ is not distribution-witnessable, let us introduce some notation for probability distributions arising from single-qubit measurements on $\rho_{ABC}(t)$. Let $P_{\phi, \chi, \psi}^{(t)}$ denote the distribution over three binary variables produced by measuring subsystem A in the basis $\{|\phi_A\rangle\langle\phi_A|, |\phi_A^\perp\rangle\langle\phi_A^\perp|\}$, subsystem B in the

basis $\{|\chi_B\rangle\langle\chi_B|, |\chi_B^\perp\rangle\langle\chi_B^\perp|\}$, and subsystem C in the basis $\{|\psi_C\rangle\langle\psi_C|, |\psi_C^\perp\rangle\langle\psi_C^\perp|\}$. We associate the outcome “0” to the first projection and “1” to the second projection in each case, so that

$$P_{\phi, \chi, \psi}^{(t)}(000) := \langle\phi_A\chi_B\psi_C|\rho_{ABC}(t)|\phi_A\chi_B\psi_C\rangle, \quad (55)$$

$$P_{\phi, \chi, \psi}^{(t)}(001) := \langle\phi_A\chi_B\psi_C^\perp|\rho_{ABC}(t)|\phi_A\chi_B\psi_C^\perp\rangle, \quad (56)$$

and so on. With $P_{\phi,\chi,\psi}^{(t)}$ defined in this way, we can consider whether or not $I_{AB}(P_{\phi,\chi,\psi}^{(t)}) \geq \mathbf{0}$. It is worth noting that

$$I_{AB}(P_{\phi,\chi,\psi}^{(t)}) = \langle \phi_A \chi_B \psi_C | I_{AB}(\rho_{ABC}(t)) | \phi_A \chi_B \psi_C \rangle. \quad (57)$$

Ultimately, we aim to show that, for some t , $I_{AB}(P_{\phi,\chi,\psi}^{(t)}) \geq \mathbf{0}$ for every choice of ϕ , χ , and ψ . Note, however, that there is redundancy in considering all such choices since, e.g., the probability vectors $P_{\phi,\chi,\psi}^{(t)}$ and $P_{\phi^\perp,\chi,\psi}^{(t)}$ are permutations of one another, so

$$I_{AB}(P_{\phi,\chi,\psi}^{(t)}) \geq \mathbf{0} \iff I_{AB}(P_{\phi^\perp,\chi,\psi}^{(t)}) \geq \mathbf{0}. \quad (58)$$

Accordingly, it suffices to demonstrate that $I_{AB}(P_{\phi,\chi,\psi}^{(t)}(000)) \geq 0$, for every ϕ , χ , and ψ . To this end, let us define

$$\iota_{AB}(t) := \min_{|\phi_A\rangle, |\chi_B\rangle, |\psi_C\rangle} I_{AB}(P_{\phi,\chi,\psi}^{(t)}(000)). \quad (59)$$

If $\iota_{AB}(t) \geq 0$, then $I_{AB}(P_{\phi,\chi,\psi}^{(t)}) \geq \mathbf{0}$ for all ϕ, χ, ψ , and the triangle-incompatibility of $\rho_{ABC}(t)$ is not distribution-witnessable (using the AB -Cut and the witnesses derived from the inequalities from Ref. [19]).

The problem with trying to determine $\iota_{AB}(t)$ directly is that the optimization is over a nonconvex set, namely the set of three-qubit pure product states. It is, however, possible to consider a relaxation of this optimization. Let S denote the set of all three-qubit states with positive partial transpose over each subsystem, that is,

$$S := \{\rho_{ABC} : \rho_{ABC}^{\top_A} \geq 0, \rho_{ABC}^{\top_B} \geq 0, \rho_{ABC}^{\top_C} \geq 0\}. \quad (60)$$

In particular, S is convex and contains the set of pure product states. Then, we define

$$\tilde{\iota}_{AB}(t) := \min_{\rho_{ABC} \in S} \text{Tr}[\rho_{ABC} I_{AB}(\rho_{ABC}(t))]. \quad (61)$$

In light of Eq. (57), we are guaranteed that

$$\iota_{AB}(t) \geq \tilde{\iota}_{AB}(t), \quad (62)$$

so non-negativity of the latter ensures non-negativity of the former.

The primary convenience of considering this relaxed optimization is that it can be formulated as a semidefinite program (SDP) [52]. The results of this optimization are plotted in Fig. 3, where rather than use the unbounded parameter t , we plot the result as a function of the amplitude of the $|011\rangle$ term, that is, as a function of $((\sqrt{t-2})/\sqrt{t})$, which is a real parameter in the interval $[1/\sqrt{3}, 1)$.

As can be seen in the figure, the value of $\tilde{\iota}_{AB}(t)$ is strictly positive when $((\sqrt{t-2})/\sqrt{t}) \gtrsim 0.82$. By Eq. (62), this

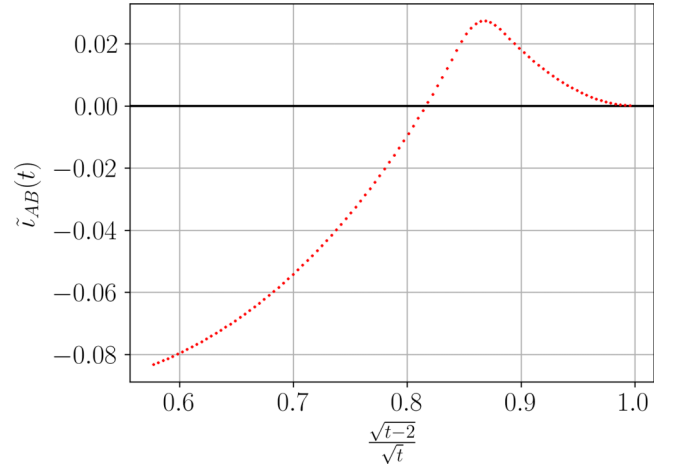


FIG. 3. The values of the semidefinite program relaxation of the problem of finding local projective measurements witnessing the nonpositivity of the AB -Cut-Bell-Wigner operators for the parameterized family of states $\rho_{ABC}(t)$. The code generating the depicted data is given in Ref. [53].

implies that the value of $\iota_{AB}(t)$ is also strictly positive in this region, and consequently that the incompatibility of states in this region are not distribution-witnessable by the AB -Cut inflation. The specific choice of t_* considered above lies in this region, so $\rho_{ABC}(t_*)$ is an example of a state that is triangle-incompatible, but for which this incompatibility is not distribution-witnessable (using the same Cut inflation and the witnesses I_{xy}).

C. The compatibility problem for mixed-states

For the case of pure three-qubit states considered above, all product and biseparable states were shown to be triangle-compatible in Sec. IV A. However, we have already seen that the analogous statement is not true for mixed-states: recall from above that the separable states $\rho^{(\text{GHZdistn})}$ and $\rho^{(\text{Wdistn})}$ that encode the classical distributions $P^{(\text{GHZ})}$ and $P^{(\text{W})}$ respectively, are triangle-incompatible. In general, any state $\rho^{(\text{distn})}$ that encodes a classical distribution in this way is triangle-incompatible if and only if the corresponding distribution is triangle-incompatible.

Since characterizing the precise set of probability distributions on three binary variables that are compatible with the triangle scenario in a quantum causal model is computationally challenging (for every nonfanout inflation it involves an infinite hierarchy of semidefinite programs [54]), a full classification of the three-qubit mixed-states that are compatible with the triangle scenario is at least as difficult.

Nonetheless, one can use the technique described here to easily derive witnesses of incompatibility for mixed quantum states.

Some of the results of Ref. [50] also provide a means for witnessing triangle-incompatibility, using ideas from the inflation technique. In fact, Ref. [50] sought to witness incompatibility for a slightly different network: the triangle supplemented by three-way shared randomness. But if one cannot realize a state with the shared randomness, then one clearly cannot realize that state without it, so any incompatibility in the former case implies triangle-incompatibility. Specifically, the witnesses considered were based on the fidelities between ρ_{ABC} and the GHZ and W states [defined, respectively, in Eqs. (51) and (52)]. One witnesses the incompatibility of ρ_{ABC} with the shared-randomness-supplemented triangle (and hence with the triangle) whenever these fidelities satisfy

$$\langle \text{GHZ} | \rho_{ABC} | \text{GHZ} \rangle \geq \frac{1 + \sqrt{3}}{4} \simeq 0.6830, \quad (63)$$

$$\langle \text{W} | \rho_{ABC} | \text{W} \rangle \geq 0.7602. \quad (64)$$

Our technique can witness triangle-incompatibilities that are not detected by the fidelity witnesses of Ref. [50]. This is the case even if we limit ourselves to the lowest level of the hierarchy of nonfanout inflations (i.e., we just consider the Cut inflation), while the bounds on the fidelities just mentioned are derived by considering higher levels of this hierarchy.

Consider the following mixed-state:

$$\omega_{ABC} = 0.3 |\psi_1\rangle\langle\psi_1| + 0.7 |0++\rangle\langle 0++|, \quad (65)$$

where

$$|\psi_1\rangle := 0.9 |000\rangle + \sqrt{0.19/2} |101\rangle + \sqrt{0.19/2} |110\rangle. \quad (66)$$

By a straightforward calculation, one can compute the operator $I_{AB}(\omega_{ABC})$ and determine that its eigenvalues are

$$\{0.788\,39, 0.195\,995, 0.035\,121\,8, -0.019\,507\,2\}, \quad (67)$$

each with multiplicity 2. The occurrence of the negative eigenvalue clearly indicates the nonpositivity of $I_{AB}(\omega_{ABC})$ and hence the triangle-incompatibility of ω_{ABC} .

On the other hand, the fidelities between ω_{ABC} and the GHZ and W states are

$$\langle \text{GHZ} | \omega_{ABC} | \text{GHZ} \rangle = 0.209, \quad (68)$$

$$\langle \text{W} | \omega_{ABC} | \text{W} \rangle = 0.233\,333, \quad (69)$$

and hence these fidelities do not satisfy the condition in Eq. (63) for witnessing incompatibility.

1. Probing triangle-incompatibility of one-parameter families of mixed-states

We saw for the case of pure three-qubit states that the boundary between compatible and incompatible states coincided exactly with the boundary between biseparable states and not biseparable states. We also saw above that in the case of mixed-states, the compatibility-incompatibility boundary is far less clear as there are separable states that are triangle-incompatible.

One method to probe this boundary further in the case of mixed-states is by adding noise to a pure-state and seeing how the positivity of a triangle-incompatibility witness behaves. Here, we consider a simple one parameter noise model that adds white noise to a given pure-state. Explicitly, for a given pure three-qubit state $|\Psi\rangle$, we consider the family indexed by $p \in [0, 1]$ defined by

$$\hat{\rho}(|\Psi\rangle, p) := p |\Psi\rangle\langle\Psi| + \frac{1-p}{8} \mathbb{1}_{ABC}, \quad (70)$$

where $\mathbb{1}_{ABC}$ is the identity on $\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C$. For any $p < 1$, $\hat{\rho}(|\Psi\rangle, p)$ is a full rank state. We have the following result:

Proposition 4. For any $|\Psi\rangle$, there exists a $q \in [3 - 2\sqrt{2}, 1)$ such that for all $0 \leq p \leq q$, $\hat{\rho}(|\Psi\rangle, p)$ is not demonstrably triangle-incompatible using the triangle-incompatibility witnesses of Eq. (44), i.e., $I_{xy}(\hat{\rho}(|\Psi\rangle, p)) \geq 0$ for each $xy \in \{AB, AC, BC\}$.

The proof is given in Appendix A 5. The result holds for any choice of the pure-state $|\Psi\rangle$ appearing in Eq. (70), which naturally includes all $|\Psi\rangle$ that are not biseparable (which we know to be demonstrably triangle-incompatible using one of the witnesses I_{xy} for $xy \in \{AB, AC, BC\}$).

In general, the value of q will be higher than $3 - 2\sqrt{2}$. For instance, if we take $|\Psi\rangle = |\text{GHZ}\rangle = (1/\sqrt{2})(|000\rangle + |111\rangle)$, making $\hat{\rho}$ a generalized three-qubit Werner state [55,56], we get that $q = \frac{1}{2}$. In this case, all the witnesses $I_{xy}(\hat{\rho}(|\text{GHZ}\rangle, p))$ are nonpositive for $p > \frac{1}{2}$, thereby witnessing the triangle-incompatibility of $\hat{\rho}(|\text{GHZ}\rangle, p)$ for these values (see Appendix A 5).

Does this tell us anything regarding the relation (or lack thereof) between the entangled-separable boundary and the boundary between triangle-compatible and triangle-incompatible states? As demonstrated in Ref. [55], the state $\hat{\rho}(|\text{GHZ}\rangle, p)$ is entangled for any $p \gtrsim 0.695\,54$ (as witnessed by the positivity of the three-tangle for those values). It follows that the entanglement boundary and triangle-incompatibility boundary are indeed distinct for this simple class of states: for $\frac{1}{2} < p < 0.6955$, the states $\hat{\rho}(|\text{GHZ}\rangle, p)$ are triangle-incompatible but not entangled. Appendix A 5 includes some details of the calculations of these q -values, also for the case where

$|\Psi\rangle = |W\rangle = (1/\sqrt{3})(|001\rangle + |010\rangle + |100\rangle)$ which produces $q \approx 0.627$.

An alternative family of Werner-like three-qubit mixed-states was studied in Ref. [57]. This single-parameter family is defined by

$$\rho^{(3,c)} := \frac{1}{8} \mathbb{1}_{ABC} + \sum_{k=X,Y,Z} \frac{1}{24} \mathbb{1}_A \otimes \sigma_B^{(k)} \otimes \sigma_C^{(k)} - \frac{c}{16} \left(\sigma_A^{(k)} \otimes \mathbb{1}_B \otimes \sigma_C^{(k)} + \sigma_A^{(k)} \otimes \sigma_B^{(k)} \otimes \mathbb{1}_C \right), \quad (71)$$

where c is a real parameter, $\sigma^{(k)}$ denote the Pauli matrices, and the subscripts indicate the subsystems they act upon. This family is interesting since it permits a local hidden variable model for projective measurements whenever $c \leq 1$ (cf. [Thm 2, 57]) and is not biseparable for $c > \frac{1}{3}(\sqrt{13} - 1) \approx 0.8685$. In particular, this means that, for $0.8685 < c < 1$, the states $\rho^{(3,c)}$ are multipartite entangled, but nevertheless, the probability distributions associated with projective measurements on $\rho^{(3,c)}$ admit local hidden variable models. If $c = 0$, one observes that the $\rho^{(3,c)}$ factorizes across the $A|BC$ partition (and moreover is maximally mixed on the A subsystem). By analogous arguments to the provided for biseparable pure-states, this state can be seen to be triangle-compatible. It turns out that this state is the only member of the above family that is all the rest are triangle-incompatible.

Proposition 5. The state $\rho^{(3,c)}$ is triangle-incompatible if and only if $c \neq 0$.

The proof is given in Appendix A 6. For this class of states then, it appears that the incompatibility-boundary has less to do with the separability than the *factorizability* of the state in question.

In sum, apart from providing further evidence that the triangle-incompatibility witnesses introduced above are broadly applicable to mixed-states, the results presented in this subsection point to the greater nuance involved in attempting to categorize the triangle-compatibility of mixed as opposed to pure-states.

V. VISIBLE NODES BEYOND QUBITS

The operator inequality in Eq. (30) was established by Hall for any finite-dimensional Hilbert space. Thus, the methodology of analyzing the positivity of the associated triangle-incompatibility witnesses remains valid in the cases where the visible nodes are not qubits. In this section, we provide a couple of examples of states on higher-dimensional systems that are triangle-incompatible.

A. Two qubits and one ququart, pure-states

Our first higher-dimensional example is to consider pure-states where $\mathcal{H}_A \cong \mathcal{H}_B \cong \mathbb{C}^2$ and $\mathcal{H}_C \cong \mathbb{C}^4$. Unlike the three-qubit case, it is readily seen that for such a choice of systems, there are triangle-compatible states beyond those that factorize across a bipartition. It suffices to note that the ququart can be conceptualized as a pair of qubits, say $C^{(1)}$ and $C^{(2)}$, and it is clear that in the triangle scenario one can prepare an entangled state on $AC^{(1)}$ and an entangled state on $BC^{(2)}$.

This of course does not imply that *any* pure qubit-qubit-ququart state can be prepared. For example, since a qubit can be isometrically embedded in a ququart, there are qubit-qubit-ququart states that are local isometry-equivalent to the three-qubit pure-states that are triangle-incompatible, and hence are themselves triangle-incompatible. However, there exist qubit-qubit-ququart states that do not reduce to three-qubit states and we now demonstrate that we can use the triangle-incompatibility witnesses presented above to prove the triangle-incompatibility of some such states, including those exhibiting GHZ-like entanglement.

To consider pure-states on this qubit-qubit-ququart system, it is possible to use the higher-dimensional generalized Schmidt decomposition given in Ref. [58]. A pure-state $|\Psi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C$ can be written as

$$|\Psi\rangle = \alpha_0 e^{i\phi_0} |000\rangle + \alpha_1 |011\rangle + \alpha_2 |101\rangle + \alpha_3 e^{i\phi_1} |102\rangle + \alpha_4 |110\rangle + \alpha_5 |111\rangle + \alpha_6 |112\rangle + \alpha_7 |113\rangle, \quad (72)$$

where $\alpha_l \in \mathbb{R}_{\geq 0}$, $\sum_l \alpha_l^2 = 1$ and $\phi_r \in [0, 2\pi)$ (see Appendix B for a summary of how this form is obtained from the general form in Ref. [58]). We then have the following:

Proposition 6. If $\rho_{ABC} = |\Psi\rangle\langle\Psi|$ where

$$|\Psi\rangle = \alpha_0 e^{i\phi_0} |000\rangle + \alpha_4 |110\rangle + \alpha_5 |111\rangle + \alpha_6 |112\rangle + \alpha_7 |113\rangle, \quad (73)$$

with $0 < \alpha_0^2 + \alpha_4^2 < 1$ (i.e., at least one of α_5 , α_6 , and α_7 is nonzero), then ρ_{ABC} is triangle-incompatible and this incompatibility is distribution-witnessable.

The proof is given in Appendix A 7 and proceeds by demonstrating that $I_{AC}(|\Psi\rangle\langle\Psi|)$ is not positive for the relevant values of the α parameters. It should be noted that the above result is consistent with known results establishing the impossibility of generating qudit graph states, such as the GHZ state, in networks with bipartite sources (see, e.g., Ref. [59]), but extends also to other local-unitary inequivalent states that exhibit GHZ-like entanglement.

B. Three qutrits, mixed-states

For the case of three qubits, we saw a number of distinctions between pure- and mixed-states vis-a-vis triangle-compatibility. Here, we give one final example in a similar vein for the case of three qutrits. In this example, we consider a pure three-qutrit state and a mixed three-qutrit state which have the same level of multipartite entanglement as quantified by the generalized geometric measure of entanglement (GGM) [60–62], where for the former, triangle-incompatibility can be demonstrated using the triangle-incompatibility witness while for the latter it cannot.

The GGM is a measure of entanglement for multipartite quantum states. For a given n -partite pure-state $|\psi\rangle$, the GGM of $|\psi\rangle$ is essentially a measure of how close $|\psi\rangle$ is to a nongenuinely multipartite entangled state. Formally, the GGM is defined to be [60–63]

$$\text{GGM}(|\psi\rangle) := 1 - \max_{|\phi\rangle} |\langle\psi|\phi\rangle|^2, \quad (74)$$

where the maximization is over all states $|\phi\rangle$ that are not genuinely multipartite entangled. For mixed-states, the GGM is given by a convex roof construction, i.e., for a mixed-state ρ , the GGM is given by

$$\text{GGM}(\rho) := \min_{\{p_i, |\psi_i\rangle\}} \sum_i p_i \text{GGM}(|\psi_i\rangle), \quad (75)$$

where the minimization is over all decompositions of ρ into convex mixtures of pure-states $|\psi_i\rangle$. In Ref. [63], the GGM was calculated for a number of mixed-states exhibiting certain symmetries. In particular, these mixed-states were obtained from specific pure-states via a certain choice of twirling operation, allowing the GGM of the former to be related to that of the latter. One example of this pure-state—mixed-state pairing is given by

$$|\Psi_{3,3}^{(3)}\rangle := \sqrt{p_0} |\Psi_0\rangle + \sqrt{p_1} |\Psi_1\rangle + \sqrt{1 - p_0 - p_1} |\Psi_2\rangle, \quad (76)$$

$$\begin{aligned} \rho_{3,3}^{(3)} := & p_0 |\Psi_0\rangle\langle\Psi_0| + p_1 |\Psi_1\rangle\langle\Psi_1| \\ & + (1 - p_0 - p_1) |\Psi_2\rangle\langle\Psi_2|, \end{aligned} \quad (77)$$

where $p_0, p_1, p_0 + p_1 \in [0, 1]$ and where $|\Psi_i\rangle$ are the three-qutrit states defined to be an equal superposition of computational basis states $|xyz\rangle$ such that $x + y + z = i \pmod{3}$, that is,

$$\begin{aligned} |\Psi_0\rangle := & \frac{1}{3} (|000\rangle + |111\rangle + |222\rangle \\ & |012\rangle + |021\rangle + |102\rangle \\ & |120\rangle + |201\rangle + |210\rangle), \end{aligned} \quad (78)$$

$$\begin{aligned} |\Psi_1\rangle := & \frac{1}{3} (|001\rangle + |010\rangle + |100\rangle \\ & |022\rangle + |202\rangle + |220\rangle \\ & |112\rangle + |121\rangle + |211\rangle), \end{aligned} \quad (79)$$

$$\begin{aligned} |\Psi_2\rangle := & \frac{1}{3} (|011\rangle + |101\rangle + |110\rangle \\ & |002\rangle + |020\rangle + |200\rangle \\ & |122\rangle + |212\rangle + |221\rangle). \end{aligned} \quad (80)$$

Let Z_3 denote the qutrit analog of the qubit Pauli- Z operator, i.e., $Z_3 = \sum_{j=0}^2 e^{(2\pi i j/3)} |j\rangle\langle j|$. For the twirling operator $\mathbf{P} : \mathcal{L}(\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C) \rightarrow \mathcal{L}(\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C)$ defined via

$$\rho \mapsto \frac{1}{3} \sum_{k=0}^2 (Z_3^k \otimes Z_3^k \otimes Z_3^k) \rho (Z_3^k \otimes Z_3^k \otimes Z_3^k)^\dagger, \quad (81)$$

where Z_3^k denotes the k th power of Z_3 , we have that $\mathbf{P}(|\Psi_{3,3}^{(3)}\rangle\langle\Psi_{3,3}^{(3)}|) = \rho_{3,3}^{(3)}$.

As a consequence of the above relation via $\mathbf{P}$, the GGM of $|\Psi_{3,3}^{(3)}\rangle$ and that of $\rho_{3,3}^{(3)}$ coincide. However, when it comes to proving the triangle-compatibility of these states by the witness I_{AB} , there is a difference between them. It turns out that $I_{AB}(\rho_{3,3}^{(3)})$, $I_{AC}(\rho_{3,3}^{(3)})$, and $I_{BC}(\rho_{3,3}^{(3)})$ have no dependence on p_0, p_1 and moreover have eigenvalues $\frac{7}{9}$ with multiplicity 3, $\frac{4}{9}$ with multiplicity 12, and $\frac{1}{9}$ also with multiplicity 12. We can thus not draw any conclusions about the triangle-compatibility of $\rho_{3,3}^{(3)}$ using this method alone.

Conversely, taking, e.g., $p_0 = 2p_1 = 0.5$, one finds that $I_{AB}(|\Psi_{3,3}^{(3)}\rangle\langle\Psi_{3,3}^{(3)}|)$ has an eigenvalue equal to -0.01348 and so $|\Psi_{3,3}^{(3)}\rangle$ is triangle-incompatible for these values of p_0, p_1 . Note that other values of p_0, p_1 also exist for which incompatibility can be demonstrated.

VI. NETWORKS BEYOND THE TRIANGLE SCENARIO

To this point, we have considered causal compatibility constraints for the triangle scenario. It is natural to ask: how readily can such constraints be derived for other causal structures? In this section, we demonstrate that the method presented in Sec. III C 1 can be applied to Cut inflations of a family of networks which includes the triangle scenario as a special case.

We begin by summarizing the method for deriving the triangle-incompatibility witnesses. From a Cut inflation G' of the triangle scenario G , a set of expressible subsets of the visible nodes of G'

$$S = \{\{A_1, B_1\}, \{A_1, C_1\}, \{B_1, C_1\}, \{A_1\}, \{B_1\}, \{C_1\}\} \quad (82)$$

is obtained. For a given state ρ_{ABC} on the visible nodes of G , by taking S to be a set of marginal contexts, we can

consider a set of states $\{\sigma_{\mathbf{X}} : \mathbf{X} \in S\}$, with the nature of the expressible sets of G' allowing each of these states to be written in terms of marginals of ρ_{ABC} . The failure of marginal compatibility of $\{\sigma_{\mathbf{X}} : \mathbf{X} \in S\}$ demonstrates the triangle-incompatibility of ρ_{ABC} and can be established by a violation of the operator inequality $\Delta(\{\sigma_{\mathbf{X}} : \mathbf{X} \in S\}) \geq 0$ proven by Hall [19] [recall Eq. (31) for the definition of Δ]. The triangle-incompatibility witness is then given by the operator $\Delta(\{\sigma_{\mathbf{X}} : \mathbf{X} \in S\})$ written in terms of the marginals of ρ_{ABC} .

There are two features of the Cut inflation of the triangle that allow the above method to work. First, the set of expressible sets S derived from the Cut inflation is such that $S = 2^{\mathbf{V}} \setminus \mathbf{V}$ for $\mathbf{V}$ an odd cardinality set of quantum systems, namely $\mathbf{V} = \{A_1, B_1, C_1\}$ in this case. The operator inequalities proven by Hall are of the form $\Delta(\{\sigma_{\mathbf{X}} : \mathbf{X} \in 2^{\mathbf{V}} \setminus \mathbf{V}\}) \geq 0$ for odd cardinality $\mathbf{V}$, so the correspondence between S and $2^{\mathbf{V}} \setminus \mathbf{V}$ is a requirement. The second feature is that *every* element of S is an expressible set in G' . This allows every term $\Delta(\{\sigma_{\mathbf{X}} : \mathbf{X} \in 2^{\mathbf{V}} \setminus \mathbf{V}\})$ to be written in terms of marginals of the state $\rho_{\mathbf{V}}$, whose compatibility with the original causal model G is being investigated, producing the desired G -incompatibility witness.

In the above case, the set $\mathbf{V}$ corresponds precisely to the set of visible nodes of the inflation G' , i.e., every subsystem specified in $\mathbf{V}$ is a single subsystem in $\text{Vnodes}(G')$. However, this is not a requirement: at least *a priori* the set $\mathbf{V}$ could contain elements that are composite systems comprising multiple visible nodes from G' . Such a scenario is not relevant when considering Cut inflations of the triangle scenario due to the small cardinality of Vnodes in this case ($|\mathbf{V}| = 3$ is the minimal case for which $\Delta(\{\sigma_{\mathbf{X}} : \mathbf{X} \in 2^{\mathbf{V}} \setminus \mathbf{V}\}) \geq 0$ is nontrivial), but for networks with larger numbers of nodes such scenarios can arise, as we demonstrate in the examples below.

Before turning to the examples, let us comment further on how the method for deriving candidate G -incompatibility witnesses works in the case where $\mathbf{V}$ contains composite systems [64]. Suppose that an inflation G' of some network G has visible nodes $\text{Vnodes}(G') = \{A_1^{[1]}, \dots, A_1^{[n]}\}$ [65] for some $n \geq 3$. Let $\{S_1, \dots, S_k\}$ denote a set partition of $\text{Vnodes}(G')$ where $k \geq 3$ is odd [66]. By taking $\mathbf{V} := \{S_1, \dots, S_k\}$ and by considering, for each $\mathbf{X} \subseteq \mathbf{V}$, the state $\sigma_{\mathbf{X}}$ to be a state on the composite system comprised of the visible nodes $\cup_{S_j \in \mathbf{X}} S_j \subseteq \text{Vnodes}(G')$, we can again consider the operator $\Delta(\{\sigma_{\mathbf{X}} : \mathbf{X} \in 2^{\mathbf{V}} \setminus \mathbf{V}\})$ as acting on the Hilbert space associated with $\text{Vnodes}(G')$. Moreover, if each element of $2^{\mathbf{V}} \setminus \mathbf{V}$ is injectable or expressible, since k is odd, it is again possible to derive an incompatibility witness from the inequality $\Delta(\{\sigma_{\mathbf{X}} : \mathbf{X} \in 2^{\mathbf{V}} \setminus \mathbf{V}\}) \geq 0$.

In the following two subsections, we consider two examples that illustrate the above method for larger numbers of visible nodes. In the first subsection, we consider the pentagon scenario, shown in Fig. 4(a), which has a

similar network structure to the triangle scenario but has 5 visible nodes instead of 3. By considering a Cut inflation of the pentagon scenario, as in Fig. 4(b), we can obtain pentagon-incompatibility witnesses both by taking $\mathbf{V}$ to be the full set of visible nodes, meaning that $|\mathbf{V}| = 5$, as well as by taking $\mathbf{V}$ to consist of composite systems, in which case $|\mathbf{V}| = 3$. In the second subsection, we consider the woven hexagon scenario, shown in Fig. 4(c), consisting of 6 visible nodes and exhibiting a higher degree of connectivity between latent and visible nodes than that of the triangle and pentagon scenarios. Using a Cut inflation for this network [cf. Fig. 4(d)], we are only able to produce an incompatibility witness by taking $\mathbf{V}$ to consist of composite systems of visible nodes (with the result that $|\mathbf{V}| = 3$).

A. Example: Pentagon scenario

Let G denote the pentagon scenario, shown in Fig. 4(a), and let G' denote the Cut inflation of G , shown in Fig. 4(b). We will start to use notation here consistent with that used below in the treatment of the general family of networks for which incompatibility witnesses can be derived. In particular, we have that the visible and latent nodes for G are

$$\begin{aligned} \text{Vnodes}(G) &= \{A_1^{[1]}, A_1^{[2]}, A_1^{[3]}, A_1^{[4]}, A_1^{[5]}\}, \\ \text{Lnodes}(G) &= \{L_1^{[1]}, L_1^{[2]}, L_1^{[3]}, L_1^{[4]}, L_1^{[5]}\}, \end{aligned} \quad (83)$$

while the visible and latent nodes for the Cut inflation G' are

$$\begin{aligned} \text{Vnodes}(G') &= \{A_1^{[1]}, A_1^{[2]}, A_1^{[3]}, A_1^{[4]}, A_1^{[5]}\}, \\ \text{Lnodes}(G') &= \{L_1^{[1]}, L_1^{[2]}, L_1^{[3]}, L_1^{[4]}, L_1^{[5]}, L_2^{[5]}\}. \end{aligned} \quad (84)$$

Note that we are considering a cut between the visible nodes $A_1^{[5]}$ and $A_1^{[1]}$ of G' , as depicted in Fig. 4(b), however Cut inflations of G can be defined for cuts introduced between any other pair of visible nodes, just as with the triangle scenario.

For the choice of labeling of the visible and latent nodes made here, the connectivity of G is given as: $L_1^{[j]}$ is the parent of $A_1^{[j]}$ and $A_1^{[j+1]}$ for each $j \in \{1, \dots, 5\}$, where any index value greater than 5 is taken modulo 5 (i.e., $L_1^{[5]}$ is the parent of both $A_1^{[5]}$ and $A_1^{[1]}$). The connectivity of G' is given as: $L_1^{[j]}$ is the parent of $A_1^{[j]}$ and $A_1^{[j+1]}$ for $j \in \{1, \dots, 4\}$, $L_1^{[5]}$ is the parent of $A_1^{[5]}$ alone and $L_2^{[5]}$ is the parent of $A_1^{[1]}$ alone. As is demonstrated in Appendix A 8, the sets

$$\{A_1^{[1]}, A_1^{[2]}, A_1^{[3]}, A_1^{[4]}\}, \quad \{A_1^{[2]}, A_1^{[3]}, A_1^{[4]}, A_1^{[5]}\} \quad (85)$$

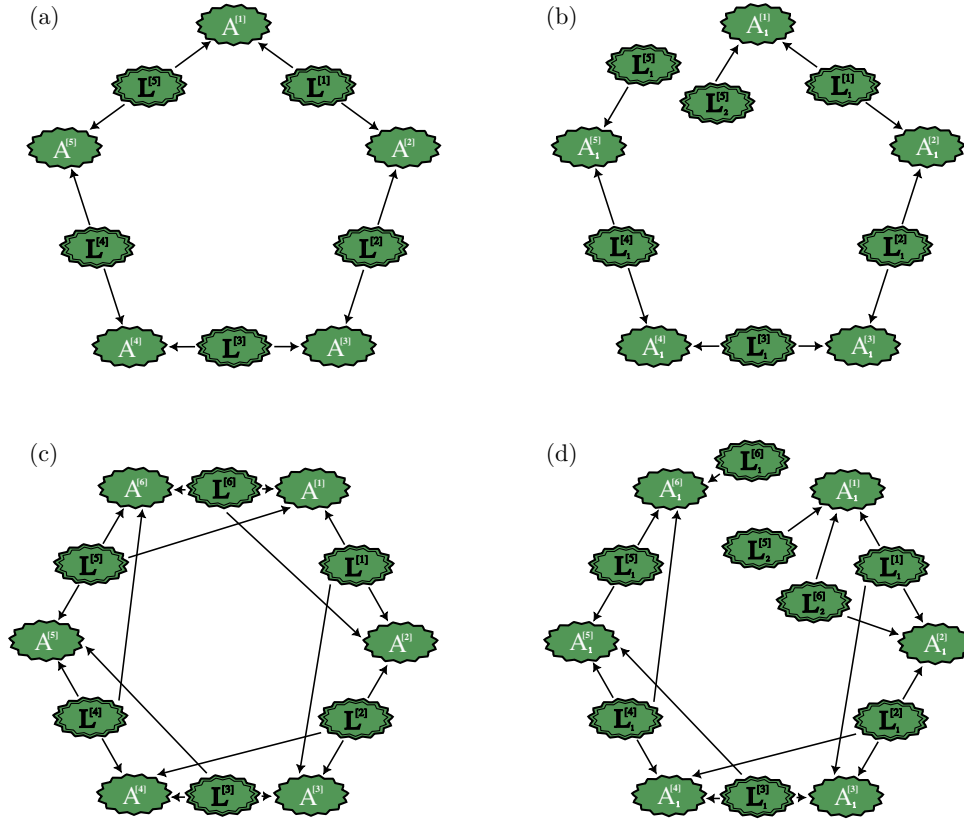


FIG. 4. (a) The pentagon scenario, corresponding to $G(5, 2)$ in the notation of the family of networks in the main text. (b) A Cut inflation of the pentagon scenario for the cut between $A_1^{[5]}$ and $A_1^{[1]}$, corresponding to $G'(5, 2, 5)$ in the main text. (c) The woven hexagon scenario, corresponding to $G(6, 3)$ in the main text. (d) A cut inflation of the woven hexagon scenario, corresponding to $G'(6, 3, 6)$ in the main text.

and all subsets thereof are injectable in G' , while the sets

$$\begin{aligned} \{A_1^{[1]}, A_1^{[2]}, A_1^{[3]}, A_1^{[5]}\}, \quad \{A_1^{[1]}, A_1^{[2]}, A_1^{[4]}, A_1^{[5]}\}, \\ \{A_1^{[1]}, A_1^{[3]}, A_1^{[4]}, A_1^{[5]}\}. \end{aligned} \quad (86)$$

and all subsets thereof are expressible.

With these sets, we can derive a number of pentagon-incompatibility witnesses. For example, taking $\mathbf{V}_1 = \{A_1^{[1]}, \dots, A_1^{[5]}\}$, we get that $|\mathbf{V}_1| = 5$ and every element of $2^{\mathbf{V}_1} \setminus \mathbf{V}_1$ is injectable or expressible. We are thus able to derive a pentagon-incompatibility witness from $\Delta(\{\sigma_{\mathbf{X}} : \mathbf{X} \in 2^{\mathbf{V}_1} \setminus \mathbf{V}_1\})$. Explicitly, if $\rho := \rho_{A[1]A[2]A[3]A[4]A[5]}$ is a state on the composite Hilbert space associated with the visible nodes of G , then the witness, denoted $I_{\mathbf{V}_1}^{\text{pent}}$, is

$$\begin{aligned} I_{\mathbf{V}_1}^{\text{pent}}(\rho) := & \mathbb{1} - \rho_{A[1]} - \rho_{A[2]} - \rho_{A[3]} - \rho_{A[4]} - \rho_{A[5]} \\ & + \rho_{A[1]A[2]} + \rho_{A[1]} \otimes \rho_{A[3]} + \rho_{A[1]} \otimes \rho_{A[4]} \\ & + \rho_{A[1]} \otimes \rho_{A[5]} + \rho_{A[2]A[3]} + \rho_{A[2]} \otimes \rho_{A[4]} \\ & + \rho_{A[2]} \otimes \rho_{A[5]} \\ & + \rho_{A[3]A[4]} + \rho_{A[3]} \otimes \rho_{A[5]} + \rho_{A[4]A[5]} \end{aligned}$$

$$\begin{aligned} & - \rho_{A[1]A[2]A[3]} - \rho_{A[1]A[2]} \otimes \rho_{A[4]} - \rho_{A[1]A[2]} \otimes \rho_{A[5]} \\ & - \rho_{A[1]} \otimes \rho_{A[3]A[4]} - \rho_{A[1]} \otimes \rho_{A[3]} \otimes \rho_{A[5]} \\ & - \rho_{A[1]} \otimes \rho_{A[4]A[5]} - \rho_{A[2]A[3]A[4]} - \rho_{A[2]A[3]} \otimes \rho_{A[5]} \\ & - \rho_{A[2]} \otimes \rho_{A[4]A[5]} - \rho_{A[3]A[4]A[5]} + \rho_{A[1]A[2]A[3]A[4]} \\ & + \rho_{A[1]A[2]A[3]} \otimes \rho_{A[5]} + \rho_{A[1]A[2]} \otimes \rho_{A[4]A[5]} \\ & + \rho_{A[1]} \otimes \rho_{A[3]A[4]A[5]} + \rho_{A[2]A[3]A[4]A[5]}. \end{aligned} \quad (87)$$

Note that the above expression makes use of the causal structure of G' : every $\sigma_{\mathbf{X}}$ for which $\mathbf{X} \in 2^{\mathbf{V}_1} \setminus \mathbf{V}_1$ contains nodes that have independent ancestry in G' , is written as a tensor product of marginals of ρ . For example, the independence arising from the cut means that $\sigma_{A_1^{[1]}A_1^{[5]}} = \rho_{A[1]} \otimes \rho_{A[5]}$ just as with the triangle scenario, but also the independence of, e.g., the visible nodes $A_1^{[2]}$ and $A_1^{[4]}$ ensure that $\sigma_{A_1^{[2]}A_1^{[4]}} = \rho_{A[2]} \otimes \rho_{A[4]}$.

If, instead, we define $\mathbf{V}_2 := \{A_1^{[1]}A_1^{[3]}, A_1^{[2]}A_1^{[5]}, A_1^{[4]}\}$, that is, by considering the partition $\{\mathcal{S}_1, \mathcal{S}_2, \mathcal{S}_3\}$ of $\text{Vnodes}(G')$, where $\mathcal{S}_1 := \{A_1^{[1]}, A_1^{[3]}\}$, $\mathcal{S}_2 := \{A_1^{[2]}, A_1^{[5]}\}$, and $\mathcal{S}_3 := \{A_1^{[4]}\}$, we obtain an *a priori* distinct

pentagon-incompatibility witness,

$$\begin{aligned} I_{V_2}^{\text{pent}}(\rho) := & \mathbb{1} - \rho_{A[1]} \otimes \rho_{A[3]} - \rho_{A[2]} \otimes \rho_{A[5]} - \rho_{A[4]} \\ & + \rho_{A[1]A[2]A[3]} \otimes \rho_{A[5]} + \rho_{A[1]} \otimes \rho_{A[3]A[4]} \\ & + \rho_{A[2]} \otimes \rho_{A[4]A[5]}. \end{aligned} \quad (88)$$

There are indeed states whose incompatibility with the pentagon scenario is witnessed by $I_{V_1}^{\text{pent}}$ and $I_{V_2}^{\text{pent}}$. Consider the five-qubit analogs to the GHZ and W states,

$$\begin{aligned} |\text{GHZ}_5\rangle &:= \frac{1}{\sqrt{2}}(|00\ 000\rangle + |11\ 111\rangle), \\ |\text{W}_5\rangle &:= \frac{1}{\sqrt{5}} \sum_{\substack{i,j,k,l,m \in \{0,1\}, \\ i+j+k+l+m=1}} |ijklm\rangle. \end{aligned} \quad (89)$$

Both $I_{V_1}^{\text{pent}}$ and $I_{V_2}^{\text{pent}}$ witness the pentagon-incompatibility of $|\text{W}_5\rangle$: $I_{V_1}^{\text{pent}}(|\text{W}_5\rangle\langle\text{W}_5|)$ has an eigenvalue of ≈ -0.3942 and $I_{V_2}^{\text{pent}}(|\text{W}_5\rangle\langle\text{W}_5|)$ has an eigenvalue of ≈ -0.1000 . However, only $I_{V_1}^{\text{pent}}$ witnesses the pentagon-incompatibility of $|\text{GHZ}_5\rangle$: $I_{V_1}^{\text{pent}}(|\text{GHZ}_5\rangle\langle\text{GHZ}_5|)$ has an eigenvalue of -0.125 while the smallest eigenvalue of $I_{V_2}^{\text{pent}}(|\text{GHZ}_5\rangle\langle\text{GHZ}_5|)$ is 0. This demonstrates that both witnesses are nontrivial and different, however the question of whether $I_{V_2}^{\text{pent}}(\rho) \not\geq 0$ implies that $I_{V_1}^{\text{pent}}(\rho) \not\geq 0$ remains open.

There are still further ways to define $\mathbf{V}$ to be different choices of set partitions of $\text{Vnodes}(G')$, which may lead to other distinct pentagon-incompatibility witnesses. Furthermore, just as with the triangle scenario, it is possible to consider different Cut inflations, of which there are now 5 in total. Between these two degrees of freedom, in choosing the Cut inflation and in choosing how to define $\mathbf{V}$, there are potentially many pentagon-incompatibility witnesses that can be obtained. Not all will be distinct as different choices of G' and $\mathbf{V}$ can lead to the same witness, and moreover, not every witness is guaranteed to be nonredundant with respect to the other witnesses. A full characterization of the set of nontrivial and nonredundant pentagon-witnesses obtained via the method presented here is left for future work.

B. Example: Woven hexagon scenario

In the pentagon scenario, each of the latent nodes has the same number of children as do the latent nodes in the triangle scenario, namely 2. It is in fact possible to derive incompatibility witnesses for network scenarios exhibiting greater connectivity, as we now demonstrate by considering the woven hexagon scenario [Fig. 4(c)]. In this scenario, every latent node has three children which impacts both the definition of what can be considered a

Cut inflation as well as the properties of the corresponding injectable and expressible sets.

The defining feature of the Cut inflations of both the triangle and pentagon scenarios is that the visible nodes between which the cut occurs, share no parents. This will be the guiding principle for defining the Cut inflations for the woven hexagon scenario here as well as the Cut inflations of the general family of networks considered below.

Let G denote the woven hexagon scenario, which has visible and latent nodes given by

$$\begin{aligned} \text{Vnodes}(G) &= \{A^{[1]}, A^{[2]}, A^{[3]}, A^{[4]}, A^{[5]}, A^{[6]}\}, \\ \text{Lnodes}(G) &= \{L^{[1]}, L^{[2]}, L^{[3]}, L^{[4]}, L^{[5]}, L^{[6]}\}. \end{aligned} \quad (90)$$

Let G' denote the Cut inflation of G for the cut between $A_1^{[6]}$ and $A_1^{[1]}$, which has visible and latent nodes

$$\begin{aligned} \text{Vnodes}(G') &= \{A_1^{[1]}, A_1^{[2]}, A_1^{[3]}, A_1^{[4]}, A_1^{[5]}, A_1^{[6]}\}, \\ \text{Lnodes}(G') &= \{L_1^{[1]}, L_1^{[2]}, L_1^{[3]}, L_1^{[4]}, L_1^{[5]}, L_1^{[6]}, L_2^{[5]}, L_2^{[6]}\}. \end{aligned} \quad (91)$$

Similarly to the pentagon scenario, the connectivity of G is given by: $L^{[j]}$ is a parent of $A^{[j+1]}, A^{[j+2]}$ for each $j \in \{1, \dots, 6\}$ with every index value greater than 6 being taken modulo 6. The connectivity of G' is given by: $L_1^{[j]}$ is a parent of $A_1^{[j]}, A_1^{[j+1]}, A_1^{[j+2]}$ for all $j \in \{1, \dots, 4\}$, $L_1^{[5]}$ is a parent of $A_1^{[5]}$ and $A_1^{[6]}$, $L_1^{[6]}$ is a parent only of $A_1^{[6]}$, $L_2^{[5]}$ is a parent only of $A_1^{[1]}$ and $L_2^{[6]}$ is a parent of $A_1^{[1]}$ and $A_1^{[2]}$. The sets

$$\{A_1^{[1]}, A_1^{[2]}, A_1^{[3]}, A_1^{[4]}\}, \quad \{A_1^{[2]}, A_1^{[3]}, A_1^{[4]}, A_1^{[5]}\}, \quad (92)$$

$$\{A_1^{[3]}, A_1^{[4]}, A_1^{[5]}, A_1^{[6]}\} \quad (93)$$

and all subsets thereof, are injectable in G' (see Appendix A 8 for details), while the sets

$$\{A_1^{[1]}, A_1^{[2]}, A_1^{[3]}, A_1^{[6]}\}, \quad \{A_1^{[1]}, A_1^{[2]}, A_1^{[5]}, A_1^{[6]}\}, \quad (94)$$

$$\{A_1^{[1]}, A_1^{[4]}, A_1^{[5]}, A_1^{[6]}\} \quad (95)$$

and all subsets thereof, are expressible.

Defining $\mathbf{V} := \{A_1^{[1]}A_1^{[6]}, A_1^{[2]}A_1^{[3]}, A_1^{[4]}A_1^{[5]}\}$, that is, with respect to the partition $\{\mathcal{S}_1, \mathcal{S}_2, \mathcal{S}_3\}$ of $\text{Vnodes}(G')$ where $\mathcal{S}_1 := \{A_1^{[1]}, A_1^{[6]}\}$, $\mathcal{S}_2 := \{A_1^{[2]}, A_1^{[3]}\}$, and $\mathcal{S}_3 := \{A_1^{[4]}, A_1^{[5]}\}$, we find that the set of contexts $2^{\mathbf{V}} \setminus \mathbf{V}$ is

$$\{A_1^{[1]}A_1^{[2]}A_1^{[3]}A_1^{[6]}, A_1^{[2]}A_1^{[3]}A_1^{[4]}A_1^{[5]}, A_1^{[1]}A_1^{[4]}A_1^{[5]}A_1^{[6]}, \quad (96)$$

$$A_1^{[1]}A_1^{[6]}, A_1^{[2]}A_1^{[3]}, A_1^{[4]}A_1^{[5]}\}, \quad (97)$$

all of which are injectable or expressible. Thus, we are in a position to derive a woven hexagon-incompatibility

witness, namely,

$$\begin{aligned} I_V^{\text{w-hex}}(\rho) := & \mathbb{1} - \rho_{A^{[1]}} \otimes \rho_{A^{[6]}} - \rho_{A^{[2]A^{[3]}} - \rho_{A^{[4]A^{[5]}}} \\ & + \rho_{A^{[1]}} \otimes \rho_{A^{[2]A^{[3]}} \otimes \rho_{A^{[6]}} + \rho_{A^{[1]}} \otimes \rho_{A^{[4]A^{[5]A^{[6]}}} \\ & + \rho_{A^{[2]A^{[3]A^{[4]A^{[5]}}}. \end{aligned} \quad (98)$$

This is nontrivial as we now show. As with the pentagon scenario, let us consider generalizations of the GHZ and W states,

$$\begin{aligned} |\text{GHZ}_6\rangle &:= \frac{1}{\sqrt{2}}(|000\,000\rangle + |111\,111\rangle), \\ |\text{W}_6\rangle &:= \frac{1}{\sqrt{6}} \sum_{\substack{ij,k,l,m,o \in \{0,1\}, \\ i+j+k+l+m+o=1}} |ijklmo\rangle. \end{aligned} \quad (99)$$

We then have that $I_V^{\text{w-hex}}(|\text{GHZ}_6\rangle\langle\text{GHZ}_6|)$ has an eigenvalue of -0.125 and $I_V^{\text{w-hex}}(|\text{W}_6\rangle\langle\text{W}_6|)$ has an eigenvalue of ≈ -0.1028 , thereby witnessing the incompatibility of these two states with the woven hexagon scenario.

Again, there are a couple of possible choices for $\mathbf{V}$ such as by taking $\mathbf{V} = \{A_1^{[1]}A_1^{[2]}, A_1^{[3]}A_1^{[4]}, A_1^{[5]}A_1^{[6]}\}$ instead.

Unlike the pentagon scenario, there is no possibility of defining $\mathbf{V}$ such that $|\mathbf{V}| = 5$: this would mean that some term in the expression $\Delta(\{\sigma_{\mathbf{X}} : \mathbf{X} \in 2^{\mathbf{V}} \setminus \mathbf{V}\})$ would correspond to a state on 5 visible nodes of G' , but G' has no injectable or expressible sets of size greater than 4.

C. Incompatibility witnesses from cut inflations of a family of networks

The above examples demonstrate that it is indeed possible to derive incompatibility witnesses for more networks than just the triangle scenario, many of which require a choice of $\mathbf{V}$ where the elements are composites of the visible nodes of the inflation DAG. Furthermore, the witnesses derived for all the examples considered so far—the triangle, pentagon, and woven hexagon scenarios—have made use of Cut inflations. In this section, we demonstrate that this extends to a family of networks that include the triangle, pentagon, and woven hexagon scenarios as special cases.

The members of the family of networks that we consider will be denoted by $G(n, l)$, where $n > l \geq 2$. The network $G(n, l)$ has visible and latent nodes given by

$$\begin{aligned} \text{Vnodes}(G(n, l)) &= \{A^{[1]}, \dots, A^{[n]}\}, \\ \text{Lnodes}(G(n, l)) &= \{L^{[1]}, \dots, L^{[n]}\} \end{aligned} \quad (100)$$

and has connectivity given by: $L^{[j]}$ is a parent of $A^{[j]}, A^{[j+1]}, \dots, A^{[j+l-1]}$ for all $j \in \{1, \dots, n\}$, where every index with value i such that $i > n$ or $i \leq 0$ is considered modulo n [67]. So defined, $G(n, l)$ has n visible nodes and

n latent nodes, with each latent node having precisely l children and each visible node having precisely l parents. With this notation, $G(3, 2)$ is the triangle scenario, $G(5, 2)$ is the pentagon scenario, and $G(6, 3)$ is the woven hexagon scenario.

Cut inflations of members of this family will be denoted $G'(n, l, j)$, where $j \in \{1, \dots, n\}$ indicates the location of the cut. As stated during the treatment of the woven hexagon scenario above, the defining feature of a Cut inflation is that the visible nodes that appear on either side of the cut do not share any parents. Accordingly, if $G'(n, l, j)$ denotes a Cut inflation of G where the cut is between $A_1^{[j]}$ and $A_1^{[j+1]}$, the visible and latent nodes of $G'(n, l, j)$ are

$$\begin{aligned} \text{Vnodes}(G'(n, l, j)) &= \{A_1^{[1]}, \dots, A_1^{[n]}\}, \\ \text{Lnodes}(G'(n, l, j)) &= \{L_1^{[1]}, \dots, L_1^{[n]}, L_2^{[n-j+2]}, \dots, L_2^{[j]}\}. \end{aligned} \quad (101)$$

The connectivity of $G'(n, l, j)$ is given by: $L_1^{[i]}$ is a parent of $A_1^{[i]}, A_1^{[i+1]}, \dots, A_1^{[i+l-1]}$ if $i \notin \{j-l+2, \dots, j\}$, $L_1^{[i]}$ is a parent of $A_1^{[i]}, A_1^{[i+1]}, \dots, A_1^{[j]}$ if $i \in \{j-l+2, \dots, j\}$, and $L_2^{[i]}$ is a parent of $A_1^{[j+1]}, A_1^{[j+2]}, \dots, A_1^{[i+l-1]}$ for $i \in \{j-l+2, \dots, j\}$. With this notation, the Cut inflations considered above for the pentagon and woven hexagon scenarios are $G(5, 2, 5)$ and $G(6, 3, 6)$ respectively.

We then have the following result:

Theorem 2. Let $k \in \mathbb{N}_{>1}$ be odd. If $n \geq (l-1)k$, then there exists a partition $\{\mathcal{S}_1, \dots, \mathcal{S}_k\}$ of $\text{Vnodes}(G'(n, l, j))$ such that, taking $\mathbf{V} := \{\mathcal{S}_1, \dots, \mathcal{S}_k\}$, all elements of $2^{\mathbf{V}} \setminus \mathbf{V}$ are injectable or expressible in $G'(n, l, j)$.

The proof is given in Appendix A 8 and consists in generalizing some of the common features of the proofs for the injectable and expressible sets for the Cut inflations of the triangle, pentagon, and woven hexagon scenarios for the general case. This theorem demonstrates that incompatibility witnesses can be found using the method presented in this work for every network in the set $\{G(n, l) | (n/(l-1)) \geq 3\}$. A thorough analysis of which of these witnesses prove fruitful for testing $G(n, l)$ -incompatibility, as well as an investigation into which other causal structures admit similar witnesses, is left for future work.

VII. DISCUSSION

Demonstrating the compatibility of a probability distribution or quantum state with a causal structure is in general a difficult task. In this article we have presented a method for witnessing the incompatibility of quantum states based on a family of quantum marginal constraints [in the form of the operator inequalities of Eq. (31)] in conjunction with

the inflation technique. We have furthermore presented an array of results that demonstrate that this method can indeed be used to make progress on problems of causal compatibility.

One of the key benefits of this approach pertains to its scalability. As demonstrated in, e.g., Ref. [20], quantum marginal problems admit a semidefinite programming formulation. Accordingly, when using the inflation technique for investigating questions of causal compatibility, one can always consider the corresponding semidefinite program (SDP). However, in the cases where a witness can be obtained by a marginal inequality, such as those in Eq. (31), there is a slight advantage in terms of computational complexity as we now describe. Denoting the product of the dimensions of the subsystems involved by D , the complexity of the SDP associated with the quantum marginal problem is $\mathcal{O}\left(D^{\frac{13}{2}}\right)$ [20]. For example, for the marginal problems derived from a choice of inflation of a causal structure with qubit visible nodes, the SDP complexity would be $\mathcal{O}(2^{(13n/2)})$, where n is the number of visible nodes in the inflation DAG. Alternatively, the complexity of finding the eigendecomposition of a $D \times D$ matrix in practice is typically stated as being $\mathcal{O}(D^3)$ (improvements to the exponent exist in certain cases). Thus, producing an incompatibility witness corresponding to an inflation DAG with n qubit visible nodes allows us to perform an incompatibility test with complexity $\mathcal{O}(2^{3n})$ or better. This is clearly not an exponential speed-up over the SDP case, but it is a speed-up nonetheless.

As a consequence of this favorable scaling, we believe the method presented here has pragmatic value. As experimental realizations of quantum networks improve (see, e.g., Refs. [68–70]), it will be increasingly important to have practical methods for verifying the structure of such networks. For example, using the methods presented above it may be possible to verify that a tomographically specified network state could not have been produced in a causal structure representing the desired network, thereby revealing a deficiency in the experimentalist’s account of the setup. Furthermore, an understanding of whether it is possible to witness incompatibility via a probability distribution arising from local measurements allows for a better appreciation of the requirements for verifying a network structure.

There are also potential benefits of the approach presented here for classical causal inference. Since the quantum compatibility problem subsumes the classical compatibility problem (as every distribution can be expressed as a diagonal density operator), a test for compatibility of quantum states is also a test for compatibility of distributions. Sometimes the more abstract problem leads to progress on the more concrete problem, so it is conceivable that investigations of the sort described here and comparisons of the classical and fully quantum causal

inference problems more generally, might ultimately yield dividends for classical causal inference.

The notion of a causal model can be generalized not just from classical theories to quantum, but to any generalized probabilistic theory (GPT) (see, e.g., [71]). Boxworld [72], the toy theory of Ref. [73], and real quantum theory [74,75] are prominent examples. These theories are generally studied as foils to quantum theory, clarifying the meaning of the latter. As such, an interesting problem for future research is to study the causal compatibility problem within generalized probabilistic theories of interest and compare to the quantum case. As emphasized in this article, if one wishes to derive such constraints using the inflation technique, then one must have some constraints coming from the marginal problem to leverage. This, therefore, motivates a study of the marginal problem in various GPTs of interest.

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DATA AVAILABILITY

The data that support the findings of this article are openly available [53].

APPENDIX A: PROOFS

This appendix contains the proofs of the results presented in Secs. III–VI.

1. Proof of Lemma 1

The proof of the following lemma uses properties of the max-divergence, some of which are provided below. The

reader is referred to the relevant sections of, e.g., Refs. [76, 77] for further details.

Let $\tilde{D}_\alpha(\cdot\|\cdot)$ denote the sandwiched Rényi relative entropy where $\alpha \in (0, 1) \cup (1, \infty)$ [78, 79]. The relevance of this relative entropy for the purposes of Lemma 1 is via its connection to the max relative entropy [80] defined via

$$D_{\max}(\rho\|\sigma) = \log_2 \inf\{\lambda \in \mathbb{R} : \rho \leq \lambda\sigma\}. \quad (\text{A1})$$

The connection between the sandwiched Rényi relative entropy and the max relative entropy is established through the following proposition:

Proposition A1 ([76]). The sandwiched Rényi relative entropy converges to the max relative entropy in the limit $\alpha \rightarrow \infty$,

$$\lim_{\alpha \rightarrow \infty} \tilde{D}_\alpha(\rho\|\sigma) = D_{\max}(\rho\|\sigma). \quad (\text{A2})$$

As a consequence of the above proposition, the max relative entropy shares a number of properties with the sandwiched Rényi relative entropies, including those stated below:

Proposition A2 ([76]). The sandwiched Rényi relative entropy $\tilde{D}_\alpha$ satisfies the following properties for every states ρ and positive semidefinite operator σ for $\alpha \in [1/2, 1) \cup (1, \infty)$.

- (1) If $\text{Tr}[\sigma] \leq \text{Tr}[\rho] = 1$, then $\tilde{D}_\alpha(\rho\|\sigma) \geq 0$.
- (2) *Faithfulness:* If $\text{Tr}[\sigma] \leq 1$, we have that $\tilde{D}_\alpha(\rho\|\sigma) = 0$ if and only if $\rho = \sigma$.
- (3) If $\rho \leq \sigma$, then $\tilde{D}_\alpha(\rho\|\sigma) \leq 0$.
- (4) For every positive semidefinite operator σ' such that $\sigma' \geq \sigma$, we have $\tilde{D}_\alpha(\rho\|\sigma) \geq \tilde{D}_\alpha(\rho\|\sigma')$.

The first three items above are of the most relevance for the proof the lemma:

Proof of Lemma 1. Let ρ_{xy} be such that $\rho_{xy} \neq \rho_x \otimes \rho_y$. Suppose for a contradiction that $\rho_{xy} \leq \rho_x \otimes \rho_y$. From the consequences of Proposition A1, we know that the max relative entropy satisfies items (1)–(3) from Proposition A2. Since ρ_{xy} and $\rho_x \otimes \rho_y$ are both quantum states and hence of unit trace, from item (1) we can conclude that $D_{\max}(\rho_{xy}\|\rho_x \otimes \rho_y) \geq 0$. From the assumption that $\rho_{xy} \neq \rho_x \otimes \rho_y$, we can conclude from item (2) that $D_{\max}(\rho_{xy}\|\rho_x \otimes \rho_y) \neq 0$ and hence must be strictly positive. However, the assumption that $\rho_{xy} \leq \rho_x \otimes \rho_y$ and item (3) imply that $D_{\max}(\rho_{xy}\|\rho_x \otimes \rho_y) \leq 0$, forming the desired contradiction. The conclusion that $\rho_{xy} \leq \rho_x \otimes \rho_y$ implies that $D_{\max}(\rho_{xy}\|\rho_x \otimes \rho_y) \leq 0$ can be seen directly from Eq. (A1) since $\rho_{xy} \leq \rho_x \otimes \rho_y$ is equivalent to $\rho_{xy} \leq$

$\lambda\rho_x \otimes \rho_y$ for $\lambda = 1$. It follows that

$$\inf\{\lambda \in \mathbb{R} : \rho_{xy} \leq \lambda\rho_x \otimes \rho_y\} \leq 1 \quad (\text{A3})$$

and so taking the logarithm produces a nonpositive value for $D_{\max}(\rho_{xy}\|\rho_x \otimes \rho_y)$. ■

2. Distribution-witnessability of W-state

Here we demonstrate that, unlike the state $\rho^{(\text{Wdistn})}$ that encodes the W distribution, the triangle-incompatibility of the state $\rho^{(\text{W})} := |\text{W}\rangle\langle\text{W}|$ with $|\text{W}\rangle = (1/\sqrt{3})(|001\rangle + |010\rangle + |100\rangle)$ is distribution-witnessable using the cut-inflation.

Recall that we can write the triangle-incompatibility witness I_{AB} as

$$I_{AB}(\rho^{(\text{W})}) = \Delta(\{\rho_X^{(\text{W})} : X \in 2^V \setminus V\}) + (\rho_A^{(\text{W})} \otimes \rho_B^{(\text{W})} - \rho_{AB}^{(\text{W})}) \otimes I_C, \quad (\text{A4})$$

where $V = \{A, B, C\}$. We have that

$$\Delta(\{\rho_X^{(\text{W})} : X \in 2^V \setminus V\}) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{3} & \frac{1}{3} & 0 & \frac{1}{3} & 0 & 0 & 0 \\ 0 & \frac{1}{3} & \frac{1}{3} & 0 & \frac{1}{3} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{3} & 0 & \frac{1}{3} & \frac{1}{3} & 0 \\ 0 & \frac{1}{3} & \frac{1}{3} & 0 & \frac{1}{3} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{3} & 0 & \frac{1}{3} & \frac{1}{3} & 0 \\ 0 & 0 & 0 & \frac{1}{3} & 0 & \frac{1}{3} & \frac{1}{3} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \quad (\text{A5})$$

and

$$\rho_A^{(\text{W})} \otimes \rho_B^{(\text{W})} - \rho_{AB}^{(\text{W})} = \begin{bmatrix} \frac{1}{9} & 0 & 0 & 0 \\ 0 & -\frac{1}{9} & -\frac{1}{3} & 0 \\ 0 & -\frac{1}{3} & -\frac{1}{9} & 0 \\ 0 & 0 & 0 & \frac{1}{9} \end{bmatrix}. \quad (\text{A6})$$

Consequently, we have that

$$\begin{aligned} \langle ++- | I_{AB}(\rho^{(W)}) | ++- \rangle \\ = \langle ++- | \Delta(\{\rho_X^{(W)} : X \in 2^V \setminus V\}) | ++- \rangle \\ + \langle ++ | \rho_A^{(W)} \otimes \rho_B^{(W)} - \rho_{AB}^{(W)} | ++ \rangle \end{aligned} \quad (A7)$$

$$= \frac{1}{12} - \frac{1}{6} \quad (A8)$$

and so the probability distribution that results from measuring each subsystem of $\rho^{(W)}$ in the X -basis is triangle-incompatible.

3. Proof of Theorem 1

Prior to proving the theorem, it is convenient to show the following lemma:

Lemma A1. If $|\omega_{AB}\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$, $|\omega_{AC}\rangle \in \mathcal{H}_A \otimes \mathcal{H}_C$ and $|\omega_{BC}\rangle \in \mathcal{H}_B \otimes \mathcal{H}_C$ are nonzero, then the sets

$$\{|\omega_{AB}\rangle \otimes |0\rangle_C, |\omega_{AB}\rangle \otimes |1\rangle_C, |\omega_{AC}\rangle \otimes |0\rangle_B, |\omega_{AC}\rangle \otimes |1\rangle_B\}, \quad (A9)$$

$$\{|\omega_{AB}\rangle \otimes |0\rangle_C, |\omega_{AB}\rangle \otimes |1\rangle_C, |\omega_{BC}\rangle \otimes |0\rangle_A, |\omega_{BC}\rangle \otimes |1\rangle_A\}, \quad (A10)$$

$$\{|\omega_{AC}\rangle \otimes |0\rangle_B, |\omega_{AC}\rangle \otimes |1\rangle_B, |\omega_{BC}\rangle \otimes |0\rangle_A, |\omega_{BC}\rangle \otimes |1\rangle_A\}, \quad (A11)$$

each contain at least three linearly independent vectors.

Proof. We demonstrate the proof for Eq. (A9); the proof for the other sets are analogous. Let $|\omega_{AB}\rangle = [a, b, c, d]^\top$ and $|\omega_{AC}\rangle = [a', b', c', d']^\top$, where at least one of a, b, c, d and at least one of a', b', c', d' are nonzero by assumption. Suppose that

$$|\omega_{AC}\rangle \otimes |0\rangle_B = \alpha |\omega_{AB}\rangle \otimes |0\rangle_C + \beta |\omega_{AB}\rangle \otimes |1\rangle_C, \quad (A12)$$

$$|\omega_{AC}\rangle \otimes |1\rangle_B = \gamma |\omega_{AB}\rangle \otimes |0\rangle_C + \delta |\omega_{AB}\rangle \otimes |1\rangle_C, \quad (A13)$$

where neither α and β nor γ and δ are both-zero. The first equation requires that b and d both be 0, while the second equation requires that both a and c be 0, forming a contradiction. It follows that at least one of $|\omega_{AC}\rangle \otimes |0\rangle_B$ and $|\omega_{AC}\rangle \otimes |1\rangle_B$ is linearly independent of $|\omega_{AB}\rangle \otimes |0\rangle_C$ and $|\omega_{AB}\rangle \otimes |1\rangle_C$. ■

Let $V := \{A, B, C\}$. A further useful fact for the proof of Theorem 1 arises from the proof of Theorem 3.2 in [21]:

for $\mathcal{H}_A \cong \mathcal{H}_B \cong \mathcal{H}_C \cong \mathbb{C}^2$, we have that

$$\Delta(\{\rho_X : X \in 2^V \setminus V\}) = \rho + \tau^{-1} \rho \tau, \quad (A14)$$

where τ is the three-qubit antiunitary defined by its action on pure-states via

$$\tau \sum_{i,j,k} \alpha_{i,j,k} |ijk\rangle = \sum_{i,j,k} (-1)^{i+j+k} \alpha_{ijk}^* |\bar{i}\bar{j}\bar{k}\rangle, \quad (A15)$$

with $i, j, k \in \{0, 1\}$ and $\bar{x} := 1 - x$.

Proof of Theorem 1. Suppose $\rho_{ABC} = |\Psi\rangle\langle\Psi|$ where $|\Psi\rangle$ is genuinely tripartite entangled, meaning that each of the two-party marginals satisfies $\rho_{xy} \neq \rho_x \otimes \rho_y$. As a consequence of Lemma 1, $\rho_A \otimes \rho_B - \rho_{AB}$, $\rho_A \otimes \rho_C - \rho_{AC}$, and $\rho_B \otimes \rho_C - \rho_{BC}$ are not positive semidefinite and hence have a eigenvector with a negative eigenvalue. Let $\omega_{xy} \in \mathcal{H}_x \otimes \mathcal{H}_y$ denote an eigenvector of $\rho_x \otimes \rho_y - \rho_{xy}$ with negative eigenvalue, for $x \neq y \in \{A, B, C\}$. As a consequence of Lemma A1, we have that

$$\begin{aligned} \dim(\text{supp}(v_{AB}^- \otimes \mathbb{1}_C) \cup \text{supp}(v_{AC}^- \otimes \mathbb{1}_B) \\ \cup \text{supp}(v_{BC}^- \otimes \mathbb{1}_A)) \geq 3. \end{aligned} \quad (A16)$$

Noting that $\tau^{-1}|\Psi\rangle$ is orthogonal to $|\Psi\rangle$, it follows from Eq. (A14) that $\dim(\text{supp}(\Delta(\{\rho_X : X \in 2^V \setminus V\}))) = 2$ (i.e., for any orthonormal basis of $\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C$ containing $|\Psi\rangle$ and $\tau^{-1}|\Psi\rangle$, the other six basis vectors are in the kernel of $\Delta(\{\rho_X : X \in 2^V \setminus V\})$). It follows that there exists a $|\Phi\rangle \in \text{supp}(v_{xy}^- \otimes \mathbb{1}_z) \cap \ker(\Delta(\{\rho_X : X \in 2^V \setminus V\}))$ for some $x, y, z \in \{A, B, C\}$ with $x \neq y \neq z \neq x$, and so the result follows from Proposition 2. ■

4. Proof of Proposition 3

Proposition 3 establishes that there exist states whose triangle-incompatibility is not distribution-witnessable. The proof of this proposition makes use of a one-parameter family of pure-states,

$$|\Psi(t)\rangle = \frac{\sqrt{t-2}}{\sqrt{t}} |100\rangle + \frac{1}{\sqrt{t}} |001\rangle + \frac{1}{\sqrt{t}} |010\rangle, \quad (A17)$$

where t is a real parameter in the interval $[3, \infty)$. These are categorized as “tri-Bell” states according to the classification of Ref. [81]. Note that the boundary of this family, at $t = 3$, is the W state of Eq. (52). We will use the notation $\rho_{ABC}(t)$ for the member of this family for a given t .

Since every element of this family of states (for finite t) fails to factorize across any bipartition, by Theorem 1, they are all incompatible with the triangle scenario. Furthermore, this incompatibility can be demonstrated using the triangle-incompatibility witness I_{AB} , as we will now see.

For $\rho_{ABC}(t)$, the eigenvalues of $I_{AB}(\rho_{ABC}(t))$ are

$$\left\{ \frac{1}{t^2}(t-2), \frac{r_1}{t^2}, \frac{r_2}{t^2}, \frac{r_3}{t^2} \right\}, \quad (\text{A18})$$

each with multiplicity 2, where r_1, r_2, r_3 are the roots of the cubic polynomial

$$f(x) = x^3 + (-t^2 + t - 2)x^2 + (-4 + 8t - 5t^2 + t^3)x + (8 - 20t + 14t^2 - 5t^3 + t^4). \quad (\text{A19})$$

For a given $t \geq 3$, the demonstration of a negative value for r_1, r_2 , or r_3 suffices to prove that $\rho_{ABC}(t)$ is triangle-incompatible. Since $I_{AB}(\rho_{ABC}(t))$ is Hermitian for all t , it must be that $r_1, r_2, r_3 \in \mathbb{R}$. Via Vieta's formula [82] (see also [83]), we get that

$$r_1 r_2 r_3 = -(8 - 20t + 14t^2 - 5t^3 + t^4). \quad (\text{A20})$$

As the quartic polynomial inside the brackets on the right-hand side is strictly positive for $t > 2$, it follows that $r_1 r_2 r_3$ is strictly negative, indicating at least one negative root. Thus $\rho_{ABC}(t)$ is triangle-incompatible for the range of values of t that we consider (i.e., $t \geq 3$). Any normalized eigenvector corresponding to a negative eigenvalue is thus a state that witnesses this incompatibility.

The fact that there exist values of t such that incompatibility of $\rho_{ABC}(t)$ is not distribution-witnessable was considered in Sec. IV B. To show that $\rho_{ABC}(t)$ for certain t is not distribution-witnessable using the AB -Cut inflation is equivalent to demonstrating that the quantity

$$\begin{aligned} & \iota_{AB}(\rho_{ABC}(t)) \\ &:= \min_{|\phi_A\rangle, |\phi_B\rangle, |\phi_C\rangle} \langle \phi_A \phi_B \phi_C | I_{AB}(\rho_{ABC}(t)) | \phi_A \phi_B \phi_C \rangle \end{aligned} \quad (\text{A21})$$

is non-negative. To do so, we consider a relaxation of the above nonconvex optimization to a convex one, namely,

$$\tilde{\iota}_{AB}(\rho_{ABC}(t)) := \min_{\rho_{ABC} \in S} \text{Tr}[\rho_{ABC} I_{AB}(\rho_{ABC}(t))], \quad (\text{A22})$$

where S denotes the set of all three-qubit states with positive partial transposes over each subsystem, that is,

$$S := \{\rho_{ABC} : \rho_{ABC}^{\top_A} \geq 0, \rho_{ABC}^{\top_B} \geq 0, \rho_{ABC}^{\top_C} \geq 0\}. \quad (\text{A23})$$

This set S contains the set of pure product states, meaning that $\iota_{AB}(t)$ is guaranteed to be lower bounded by $\tilde{\iota}_{AB}(t)$. As discussed previously, the latter quantity is indeed non-negative, e.g., when $t \geq 7$.

5. Proof of Proposition 4

Proof of Proposition 4. Let us write $\rho_{ABC} = |\Psi\rangle\langle\Psi|$ so $\hat{\rho}(|\Psi\rangle, p) = p\rho_{ABC} + ((1-p)/8)\mathbb{1}_{ABC}$. For convenience, we will at times write $\hat{\rho}$ for $\hat{\rho}(|\Psi\rangle, p)$. By linearity, we see that

$$\begin{aligned} \Delta(\{\hat{\rho}_{\mathbf{X}} : \mathbf{X} \in 2^{\mathbf{V}} \setminus \mathbf{V}\}) &= p\Delta(\{\rho_{\mathbf{X}} : \mathbf{X} \in 2^{\mathbf{V}} \setminus \mathbf{V}\}) \\ &+ (1-p)\Delta\left(\left\{\frac{\mathbb{1}_{\mathbf{X}}}{2^{|\mathbf{X}|}} : \mathbf{X} \in 2^{\mathbf{V}} \setminus \mathbf{V}\right\}\right). \end{aligned} \quad (\text{A24})$$

Furthermore, recalling Eq. (36), we have that $\Delta(\{\frac{\mathbb{1}_{\mathbf{X}}}{2^{|\mathbf{X}|}} : \mathbf{X} \in 2^{\mathbf{V}} \setminus \mathbf{V}\}) = \frac{1}{4}\mathbb{1}_{ABC}$. We demonstrate that there exists a $q \in [3 - 2\sqrt{2}, 1)$ such that $I_{AB}(\hat{\rho}(|\Psi\rangle, p)) \geq 0$ for all $0 \leq p \leq q$; the proofs for the other triangle-incompatibility witnesses proceed analogously, and the result is obtained by taking the minimal value of q for the three cases.

Since

$$\hat{\rho}_A \otimes \hat{\rho}_B = (p\rho_A + \frac{1-p}{2}\mathbb{1}_A) \otimes (p\rho_B + \frac{1-p}{2}\mathbb{1}_B) \quad (\text{A25})$$

$$= p^2\rho_A \otimes \rho_B + \frac{p(1-p)}{2}\rho_A \otimes \mathbb{1}_B + \frac{p(1-p)}{2}\mathbb{1}_A \otimes \rho_B + \frac{(1-p)^2}{4}\mathbb{1}_{AB} \quad (\text{A26})$$

$$\hat{\rho}_{AB} = p\rho_{AB} + \frac{(1-p)}{4}\mathbb{1}_{AB} \quad (\text{A27})$$

and $I_{AB}(\hat{\rho}) = \Delta(\{\hat{\rho}_{\mathbf{X}} : \mathbf{X} \in 2^{\mathbf{V}} \setminus \mathbf{V}\}) + \hat{\rho}_A \otimes \hat{\rho}_B - \hat{\rho}_{AB}$, we get that

$$\begin{aligned} I_{AB}(\hat{\rho}) &= p\Delta(\{\rho_{\mathbf{X}} : \mathbf{X} \in 2^{\mathbf{V}} \setminus \mathbf{V}\}) + \frac{1-p}{4}\mathbb{1}_{ABC} + p^2\rho_A \otimes \rho_B \otimes \mathbb{1}_C + \frac{p(1-p)}{2}\rho_A \otimes \mathbb{1}_{BC} \\ &+ \frac{p(1-p)}{2}\mathbb{1}_{AC} \otimes \rho_B + \frac{(1-p)^2}{4}\mathbb{1}_{ABC} - p\rho_{AB} \otimes \mathbb{1}_C - \frac{(1-p)}{4}\mathbb{1}_{ABC} \end{aligned} \quad (\text{A28})$$

$$\begin{aligned} &= p\Delta(\{\rho_{\mathbf{X}} : \mathbf{X} \in 2^{\mathbf{V}} \setminus \mathbf{V}\}) + p^2\rho_A \otimes \rho_B \otimes \mathbb{1}_C + \frac{p(1-p)}{2}\rho_A \otimes \mathbb{1}_{BC} + \frac{p(1-p)}{2}\mathbb{1}_{AC} \otimes \rho_B \\ &+ \frac{(1-p)^2}{4}\mathbb{1}_{ABC} - p\rho_{AB} \otimes \mathbb{1}_C. \end{aligned} \quad (\text{A29})$$

Noting that a sufficient condition for $A - B \geq 0$ for A and B positive semidefinite matrices is that the maximal eigenvalue of B is less than or equal to the minimal eigenvalue of A , we see that $((1-p)^2/4)\mathbb{1}_{ABC} - p\rho_{AB} \otimes \mathbb{1}_C \geq 0$ is guaranteed at least when $\frac{1}{4}(1-p)^2 - p \geq 0$, i.e., for $0 \leq p \leq 3 - 2\sqrt{2}$. It follows that $I_{AB}(\hat{\rho})$ is guaranteed to be positive semidefinite at least for $0 \leq p \leq q := 3 - 2\sqrt{2}$. The same reasoning holds for I_{AC} and I_{BC} with the same value of q . ■

The above proof establishes a lower bound for q that is generally not tight for a given pure-state $|\Psi\rangle$. For $\hat{\rho}(|\text{GHZ}\rangle, p)$, the eigenvalues of $I_{xy}(\hat{\rho})$ are the same for all $xy \in \{AB, AC, BC\}$ and are given by $\frac{1}{4}\{1, 1 \pm 2p\}$, where the first has multiplicity 4 and the others multiplicity 2. Thus, for $p \leq \frac{1}{2}$, the $I_{xy}(\hat{\rho})$ are all positive.

For $\hat{\rho}(|W\rangle, p)$, the eigenvalues of $I_{xy}(\hat{\rho})$ are the same for all $xy \in \{AB, AC, BC\}$ and are given by

$$\frac{1}{36} \left\{ 9 - p^2, 9 - 6p + p^2, 9 + 3p \pm \sqrt{297p^2 + 6p^3 + p^4} \right\}, \quad (\text{A30})$$

each with multiplicity 2. These eigenvalues are all positive whenever $9 + 3p \geq \sqrt{297p^2 + 6p^3 + p^4}$, which occurs for $p \lesssim 0.627$.

6. Proof of Proposition 5

Any three-qubit mixed-state can be written as [84]

$$\begin{aligned} \rho_{ABC} = & \frac{1}{8} \mathbb{1}_{ABC} + \sum_{i,j,k=X,Y,Z} a_i \sigma_A^i + b_j \sigma_B^j + c_k \sigma_C^k + d_{ij} \sigma_A^i \\ & \otimes \sigma_B^j + e_{ik} \sigma_A^i \otimes \sigma_C^k + f_{jk} \sigma_B^j \otimes \sigma_C^k + g_{ijk} \sigma_A^i \\ & \otimes \sigma_B^j \otimes \sigma_C^k, \end{aligned} \quad (\text{A31})$$

where the σ^l for $l = X, Y, Z$ denote the Pauli operators and where all the coefficients are real (recall that the Pauli matrices form an operator basis for the real vector space of Hermitian operators). Each term in the above expression is to be understood as an operator $\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C$ —identity operators have been omitted for brevity.

Substituting the expression for ρ_{ABC} into Eq. (41) and the corresponding equations for the AC and BC triangle-incompatibility witnesses, we get that

$$I_{AB}(\rho) = \frac{1}{4} \mathbb{1}_{ABC} + \sum_{i,j,k=X,Y,Z} 16a_i b_j \sigma_A^i \otimes \sigma_B^j + 2e_{ik} \sigma_A^i \otimes \sigma_C^k + 2f_{jk} \sigma_B^j \otimes \sigma_C^k, \quad (\text{A32})$$

$$I_{AC}(\rho) = \frac{1}{4} \mathbb{1}_{ABC} + \sum_{i,j,k=X,Y,Z} 2d_{ij} \sigma_A^i \otimes \sigma_B^j + 16a_i c_k \sigma_A^i \otimes \sigma_C^k + 2f_{jk} \sigma_B^j \otimes \sigma_C^k, \quad (\text{A33})$$

$$I_{BC}(\rho) = \frac{1}{4} \mathbb{1}_{ABC} + \sum_{i,j,k=X,Y,Z} 2d_{ij} \sigma_A^i \otimes \sigma_B^j + 2e_{ik} \sigma_A^i \otimes \sigma_C^k + 16b_j c_k \sigma_B^j \otimes \sigma_C^k. \quad (\text{A34})$$

For the family of states $\rho^{(3,c)}$, we see that $a_i = b_j = c_k = 0$ for all i, j, k and that $d_{ij} = -(c/16)\delta_{ij}$, $e_{ik} = -(c/16)\delta_{ik}$, and $f_{jk} = \frac{1}{24}\delta_{jk}$. Thus,

$$I_{AB}(\rho^{(3,c)}) = \frac{1}{4} \mathbb{1}_{ABC} + \sum_{k=X,Y,Z} \frac{1}{12} \sigma_B^k \otimes \sigma_C^k - \frac{c}{8} \sigma_A^i \otimes \sigma_C^k \quad (\text{A35})$$

$$= \begin{bmatrix} \frac{1}{3} - \frac{c}{8} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{c}{8} + \frac{1}{6} & \frac{1}{6} & 0 & -\frac{c}{4} & 0 & 0 & 0 \\ 0 & \frac{1}{6} & \frac{1}{6} - \frac{c}{8} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{c}{8} + \frac{1}{3} & 0 & 0 & -\frac{c}{4} & 0 \\ 0 & -\frac{c}{4} & 0 & 0 & \frac{c}{8} + \frac{1}{3} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{6} - \frac{c}{8} & \frac{1}{6} & 0 \\ 0 & 0 & 0 & -\frac{c}{4} & 0 & \frac{1}{6} & \frac{c}{8} + \frac{1}{6} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{3} - \frac{c}{8} \end{bmatrix}. \quad (\text{A36})$$

This operator has eigenvalues $\frac{1}{24}(8 - 3c)$ and $\frac{1}{24}(4 + 3c \pm 2\sqrt{4 + 6c + 9c^2})$, the first with multiplicity 4 and the others each with multiplicity 2. It is readily verified that $4 + 3c - 2\sqrt{4 + 6c + 9c^2}$ is strictly negative for $c \neq 0$, establishing the result.

7. Proof of Proposition 6

For $\rho_{ABC} = |\Psi\rangle\langle\Psi|$, where

$$|\Psi\rangle = \alpha_0 e^{i\phi_0} |000\rangle + \alpha_4 |110\rangle + \alpha_5 |111\rangle + \alpha_6 |112\rangle + \alpha_7 |113\rangle, \quad (\text{A37})$$

we have that

$$I_{AC}(\rho_{ABC}) = \begin{bmatrix} \Gamma_1 & \mathbf{0} & \mathbf{0} & e^{i\phi_0} \alpha_0 \alpha_4 \mathbb{1} \\ \mathbf{0} & \Gamma_2 & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & -\Gamma_2 & \mathbf{0} \\ e^{-i\phi_0} \alpha_0 \alpha_4 \mathbb{1} & \mathbf{0} & \mathbf{0} & \mathbb{1} - \Gamma_1 \end{bmatrix}, \quad (\text{A38})$$

where here $\mathbb{1}$ is the 4×4 identity matrix and

$$\Gamma_1 := \begin{bmatrix} \alpha_0^4 + (\alpha_4^2 - 1)\alpha_0^2 - \alpha_4^2 + 1 & (\alpha_0^2 - 1)\alpha_4\alpha_5 & (\alpha_0^2 - 1)\alpha_4\alpha_6 & (\alpha_0^2 - 1)\alpha_4\alpha_7 \\ (\alpha_0^2 - 1)\alpha_4\alpha_5 & (\alpha_0^2 - 1)(\alpha_5^2 - 1) & (\alpha_0^2 - 1)\alpha_5\alpha_6 & (\alpha_0^2 - 1)\alpha_5\alpha_7 \\ (\alpha_0^2 - 1)\alpha_4\alpha_6 & (\alpha_0^2 - 1)\alpha_5\alpha_6 & (\alpha_0^2 - 1)(\alpha_6^2 - 1) & (\alpha_0^2 - 1)\alpha_6\alpha_7 \\ (\alpha_0^2 - 1)\alpha_4\alpha_7 & (\alpha_0^2 - 1)\alpha_5\alpha_7 & (\alpha_0^2 - 1)\alpha_6\alpha_7 & (1 - \alpha_0^2)(1 - \alpha_7^2) \end{bmatrix}, \quad (\text{A39})$$

$$\Gamma_2 := \begin{bmatrix} -\alpha_0^2(1 - \alpha_0^2 - \alpha_4^2) & \alpha_0^2\alpha_4\alpha_5 & \alpha_0^2\alpha_4\alpha_6 & \alpha_0^2\alpha_4\alpha_7 \\ \alpha_0^2\alpha_4\alpha_5 & \alpha_0^2\alpha_5^2 & \alpha_0^2\alpha_5\alpha_6 & \alpha_0^2\alpha_5\alpha_7 \\ \alpha_0^2\alpha_4\alpha_6 & \alpha_0^2\alpha_5\alpha_6 & \alpha_0^2\alpha_6^2 & \alpha_0^2\alpha_6\alpha_7 \\ \alpha_0^2\alpha_4\alpha_7 & \alpha_0^2\alpha_5\alpha_7 & \alpha_0^2\alpha_6\alpha_7 & \alpha_0^2\alpha_7^2 \end{bmatrix}. \quad (\text{A40})$$

By inspection, one notices that

$$\langle 010 | I_{AC}(\rho_{ABC}) | 010 \rangle = -\alpha_0^2(1 - \alpha_0^2 - \alpha_4^2), \quad (\text{A41})$$

which is negative whenever $0 < \alpha_0^2 + \alpha_4^2 < 1$.

8. Proof of Theorem 2

In this appendix, we prove Theorem 2 regarding Cut inflations $G'(n, l, j)$ of the networks $G(n, l)$ where $n > l \geq 2$. Recall that $G(n, l)$ has visible and latent nodes

$$\begin{aligned} \text{Vnodes}(G(n, l)) &= \{A^{[1]}, \dots, A^{[n]}\}, \\ \text{Lnodes}(G(n, l)) &= \{L^{[1]}, \dots, L^{[n]}\}, \end{aligned} \quad (\text{A42})$$

while $G'(n, l, j)$ has visible and latent nodes,

$$\begin{aligned} \text{Vnodes}(G'(n, l, j)) &= \{A_1^{[1]}, \dots, A_1^{[n]}\}, \\ \text{Vnodes}(G'(n, l, j)) &= \{L_1^{[1]}, \dots, L_1^{[j-l+2]}, L_2^{[j-l+3]}, \dots, L_2^{[j]}\}. \end{aligned} \quad (\text{A43})$$

With this choice of notation, along with the fact that every index value greater than n or less than or equal to 0 is taken modulo n , it is easy to see that any proof of involving injectable and expressible set of $G'(n, l, j)$ can quickly become heavily entrenched in keeping track of the

subscript and superscript labeling of nodes. To ease the notational burden, we introduce some further terminology and notation and make some simplifying choices.

The main simplifying choice is that we will only consider the Cut inflation $G'(n, l, n)$, that is, the Cut inflation with the cut between the visible node $A_1^{[n]}$ and $A_1^{[1]}$ from now on. The proof for any other choice of cut proceeds analogously: by making the substitution $[t] \mapsto [t - j]$ for every superscript (with the usual convention of index values modulo n), the case of the Cut inflation $G'(n, l, j)$ is mapped to the case $G'(n, l, n)$ that we consider here.

Next, it will be convenient to consider the set $\text{Lnodes}(G'(n, l, n))$ equipped with the total order given by

$$L_2^{[n-l+2]} < L_2^{[n-l+3]} < \dots < L_2^{[n]} < L_1^{[1]} < L_1^{[2]} < \dots < L_1^{[n]}. \quad (\text{A44})$$

We will call a subset $X' \subseteq \text{Lnodes}(G'(n, l, n))$ *totally adjacent* with respect to the above total order, if it possible to write the elements of X' as a sequence $x'_1, \dots, x'_{|X'|}$ such that (i) $x'_1 < x'_2 < \dots < x'_{|X'|}$ in the order of Eq. (A44) and (ii) for each $t \in \{1, \dots, |X'| - 1\}$, there does not exist a $v \in \text{Lnodes}(G'(n, l, n))$ such that $x'_t < v < x'_{t+1}$. The sequence $x'_1, \dots, x'_{|X'|}$ will be called the *adjacency sequence* of X' .

We will also make use of the notation $\text{Anc}_{G'(n, l, j)}(\mathbf{U}') \subseteq \text{Lnodes}(G'(n, l, j))$ to denote the set of ancestors in $G'(n, l, j)$ for $\mathbf{U}' \subseteq \text{Vnodes}(G'(n, l, j))$.

Finally, let us recall the definition of injectable and expressible sets. For an inflation G' of a causal model G , a subset $U' \subseteq \text{Vnodes}(G')$ is *injectable* if there exists a subset $U \subseteq \text{Vnodes}(G)$ such that U' and U are the same up to copy-indices and moreover the ancestral subgraph of U' in G' , denoted $\text{ansubgraph}_{G'}(U')$, is the same up to copy-indices as the ancestral subgraph of U in G , denoted $\text{ansubgraph}_G(U)$. Furthermore, a subset $U' \subseteq \text{Vnodes}(G')$ is *ai-expressible* if it can be written as the union of injectable sets that are ancestrally independent. The notion of ai-expressibility is a special case of the general notion of expressible set (c.f. [15]), however, as we require neither the more general notion here nor to distinguish between the different cases, we drop the “ai-” from the terminology and refer to the sets simply as “expressible.” Any subset of an injectable or expressible set is also injectable or expressible.

As we will be considering injectable and expressible sets for the inflation $G'(n, l, n)$, let us recall the connectivity of this model,

- (a) every latent node $L_2^{[s]}$, where $s \in \{n - l + 2, \dots, n\}$ is the parent of $A_1^{[1]}, \dots, A_1^{[s+l-1]}$,
- (b) every latent node $L_1^{[s]}$, where $s \in \{1, \dots, n - l + 1\}$, is the parent of $A_1^{[s]}, \dots, A_1^{[s+l-1]}$,
- (c) every latent node $L_1^{[s]}$, where $s \in \{n - l + 2, \dots, n\}$, is the parent of $A_1^{[s]}, \dots, A_1^{[n]}$.

Before proving the theorem, we consider the following lemmata:

Lemma A2. Let $U' \subseteq \text{Vnodes}(G'(n, l, n))$ be nonempty. Suppose that $X' := \text{Anc}_{G'(n, l, n)}(U')$ is totally adjacent with respect to the order on $\text{Lnodes}(G'(n, l, n))$ [i.e., Eq. (A44)] with adjacency sequence $x'_1, \dots, x'_{|X'|}$. Then either

- (a) $x'_1 = L_2^{[s]}$ and $x'_{|X'|} = L_1^{[s+|X'|-1]}$ for some $s \in \{n - l + 2, \dots, n\}$ or
- (b) $x'_1 = L_1^{[s]}$ and $x'_{|X'|} = L_1^{[s+|X'|-1]}$ for some $s \in \{1, \dots, n - l + 1\}$.

In either case, $U' \subseteq \{A_1^{[s+l-1]}, \dots, A_1^{[s+|X'|-1]}\}$ for the relevant value of s .

Proof. Let $U' \subseteq \text{Vnodes}(G'(n, l, n))$ be nonempty and $X' := \text{Anc}_{G'(n, l, n)}(U')$ be totally adjacent with respect to the order on $\text{Lnodes}(G'(n, l, n))$. Since U' contains at least one visible node and since each visible node in $G'(n, l, n)$ has at least l parents, $|X'| \geq l$. Note that $\text{Lnodes}(G'(n, l, n))$ contains $l - 1$ elements with a subscript “2,” namely $L_2^{[n-l+2]}, \dots, L_2^{[n]}$, meaning that any totally adjacent subset of $\text{Lnodes}(G'(n, l, n))$ containing

at least l elements has adjacency sequence that must terminate with an element with a subscript “1.” The possible cases then split into the cases (a) and (b) in the statement of the lemma.

Due to the assumption of total adjacency for X' , the sequence $x'_1, \dots, x'_{|X'|}$ contains $|X'|$ adjacent elements in the ordering of Eq. (A44). If, as in case (a), the sequence commences with $x_1 = L_2^{[s]}$ for some $s \in \{n - l + 2, \dots, n\}$, then the sequence is

$$L_2^{[s]}, L_2^{[s+1]}, \dots, L_2^{[n]}, L_1^{[1]}, L_1^{[2]}, \dots, L_1^{[s+|X'|-1]}. \quad (\text{A45})$$

If, as in case (b), the sequence commences with $L_1^{[s]}$ for $s \in \{1, \dots, n - l + 1\}$ [note that if $s \in \{n - l + 2, \dots, n\}$, then the sequence could not be at least l elements long and totally adjacent with respect to the order Eq. (A44)], then the sequence is

$$L_1^{[s]}, \dots, L_1^{[s+|X'|-1]}. \quad (\text{A46})$$

We now show that $U' \subseteq \{A_1^{[s+l-1]}, \dots, A_1^{[s+|X'|-1]}\}$. If $\{A_1^{[s+l-1]}, \dots, A_1^{[s+|X'|-1]}\} = \text{Vnodes}(G'(n, l, n))$, then this is trivially true so we assume that $\{A_1^{[s+l-1]}, \dots, A_1^{[s+|X'|-1]}\} \neq \text{Vnodes}(G'(n, l, n))$ from now on. In particular, this means that either $s \neq n - l + 2$, resulting in $A_1^{[s+l-1]} = A_1^{[r]}$ for some $r > 1$ after applying the convention on the indices or $s \neq n - |X'| + 1$, resulting in $A_1^{[s+|X'|-1]} = A_1^{[r]}$ for some $r < n$, or both.

We proceed by contradiction. Suppose $U' \not\subseteq \{A_1^{[s+l-1]}, \dots, A_1^{[s+|X'|-1]}\}$ and recall that either (a') $X' = \{L_2^{[s]}, L_2^{[s+1]}, \dots, L_2^{[n]}, L_1^{[1]}, L_1^{[2]}, \dots, L_1^{[s+|X'|-1]}\}$ for some $s \in \{n - l + 2, \dots, n\}$, or (b') $X' = \{L_1^{[s]}, L_1^{[s+1]}, \dots, L_1^{[s+|X'|-1]}\}$ for some $s \in \{1, \dots, n - l + 1\}$. In case (a'), if $s \neq n - |X'| + 1$ and there exists an $A_1^{[t]} \in U'$ with $t \in \{s + |X'|, \dots, n\}$ [85], then since $L_1^{[t]}$ is a parent of $A_1^{[t]}$, this would require that $L_1^{[t]} \in X'$, forming a contradiction. If $s \neq n - l + 2$ and there exists an $A_1^{[t]} \in U'$ with $t \in \{1, \dots, s + l - 2\}$, then since $L_2^{[t-l+1]}$ is a parent of $A_1^{[t]}$, this would require that $L_2^{[t-l+1]} \in X'$ which also forms a contradiction. Since at least one of these two possibilities must occur under the assumption that $\{A_1^{[s+l-1]}, \dots, A_1^{[s+|X'|-1]}\} \neq \text{Vnodes}(G'(n, l, n))$, this completes the case for (a').

The situation for (b') is analogous. If $s \neq n - |X'| + 1$ and there exists an $A_1^{[t]} \in U'$ with $t \in \{s + |X'|, \dots, n\}$, then since $L_1^{[t]}$ is a parent of $A_1^{[t]}$, this would require that $L_1^{[t]} \in X'$, forming a contradiction, same as above. If $s \neq n - l + 2$ and there exists an $A_1^{[t]} \in U'$ with $t \in \{1, \dots, s + l - 2\}$, then either (I) $A_1^{[t]}$ has a parent $L_2^{[t-l+1]}$ if $t \in \{1, \dots, l - 1\}$ or (II) $A_1^{[t]}$ has a parent $L_1^{[t-l+1]}$ if $t \in \{l, \dots, s + l - 2\}$. In case (I), this would require that

$L_2^{[t-l+1]} \in X'$ and in case (II), this would require that $L_1^{[t-l+1]} \in X'$, both of which form contradictions. ■

Lemma A3. Let $\text{Lnodes}(G'(n, l, n))$ be equipped with the ordering of Eq. (A44) and let $U' \subseteq \text{Vnodes}(G'(n, l, n))$. If $\text{Anc}_{G'(n, l, n)}(U')$ is totally adjacent with respect to the ordering on $\text{Lnodes}(G'(n, l, n))$ and if $|\text{Anc}_{G'(n, l, n)}(U')| = n$, then U' is an injectable set.

Proof. Let $U' \subseteq \text{Vnodes}(G'(n, l, n))$ be such that $X' := \text{Anc}_{G'(n, l, n)}(U')$ is totally ordered and that $|X'| = n$. From Lemma A2, we know that either $X' = \{L_2^{[s]}, \dots, L_2^{[n]}, L_1^{[1]}, \dots, L_1^{[n+s-1]}\}$ for some $s \in \{n-l+2, \dots, n\}$ or $X' = \{L_1^{[s]}, \dots, L_1^{[n+s-1]}\}$ for some $s \in \{1, \dots, n-l+1\}$, and moreover that $U' \subseteq \{A_1^{[s+l-1]}, \dots, A_1^{[n+s-1]}\}$ for the relevant value of s . Since any subset of an injectable set is also injectable, it suffices to show that $W' := \{A_1^{[s+l-1]}, \dots, A_1^{[n+s-1]}\}$ is injectable in $G'(n, l, n)$.

Recall that $W' \subseteq \text{Vnodes}(G'(n, l, n))$ is injectable if and only if there exists a subset $W \subseteq \text{Vnodes}(G(n, l))$ such that $W' \sim W$ and $\text{ansubgraph}_{G'(n, l, n)}(W') \sim \text{ansubgraph}_{G(n, l)}(W)$, where $\sim$ denotes sameness up to copy-index and where $\text{ansubgraph}_{G'(n, l, n)}(W')$ denotes the ancestral subgraph of W' in $G'(n, l, n)$ [similarly for $\text{ansubgraph}_{G(n, l)}(W)$]. Defining $W := \{A_1^{[s+l-1]}, \dots, A_1^{[n+s-1]}\}$, we have that $W' \sim W$.

Next, recall that $\text{Lnodes}(G(n, l)) = \{L_1^{[1]}, \dots, L_1^{[n]}\}$. Due to the choice of ordering in Eq. (A44) and to the fact that $|X'| = n$, we have that $X' \sim \text{Lnodes}(G(n, l))$ in either case for X' . Since each visible node $A_1^{[l]}$ in $G(n, l)$ has parents $L_1^{[t-l+1]}, L_1^{[t-l+2]}, \dots, L_1^{[t]}$, we see that $X := \text{Anc}_{G(n, l)}(W) = \{L_1^{[s]}, \dots, L_1^{[n+s-1]}\} = \text{Lnodes}(G(n, l))$. Hence, we have that $X' \sim X$. Recall that, by definition of inflation, the ancestral subgraph of any single visible node in an inflation is the same up to copy-indices as the ancestral subgraph of the corresponding visible node in the original causal model. Since X' contains no two elements with a common superscript but different subscripts, any common parents of any subset of visible nodes of W' will be the unique latent nodes with the relevant superscript, which ensures that $\text{ansubgraph}_{G'(n, l, n)}(W') \sim \text{ansubgraph}_{G(n, l)}(W)$. ■

Lemma A4. Let $\text{Lnodes}(G'(n, l, n))$ be given the ordering in Eq. (A44). Let $U_1, U_2 \subseteq \text{Vnodes}(G'(n, l, n))$. If

- (1) $A_1^{[n]} \in U_1$ and $A_1^{[1]} \in U_2$,
- (2) $\text{Anc}_{G'(n, l, n)}(U_1)$ and $\text{Anc}_{G'(n, l, n)}(U_2)$ are totally adjacent, and
- (3) $\text{Anc}_{G'(n, l, n)}(U_1)$ and $\text{Anc}_{G'(n, l, n)}(U_2)$ form a set partition of $\text{Lnodes}(G'(n, l, n))$,

then $U_1 \cup U_2$ is an expressible set.

Proof. Let $U_1, U_2 \subseteq \text{Vnodes}(G'(n, l, n))$ be such that $A_1^{[n]} \in U_1$ and $A_1^{[1]} \in U_2$, $X_1' := \text{Anc}_{G'(n, l, n)}(U_1)$ and $X_2' := \text{Anc}_{G'(n, l, n)}(U_2)$ are totally adjacent, and X_1' and X_2' form a set partition of $\text{Lnodes}(G'(n, l, n))$. Recall that for $U_1 \cup U_2$ to be expressible, it suffices to have that U_1 and U_2 are injectable and are ancestrally independent. However, the latter requirement follows directly from the assumption that X_1' and X_2' form a set partition of $\text{Lnodes}(G'(n, l, n))$ (recall that mutual exclusivity is a requirement in the definition of set partition).

To show that U_1 and U_2 are indeed injectable, we first note the following bounds on X_1' and X_2' . Since $A_1^{[n]} \in U_1$, it must be the case that $|X_1'| \geq l$ since $A_1^{[n]}$ has l parents in $G'(n, l, n)$. By the same reasoning $|X_2'| \geq l$. Since $|\text{Lnodes}(G'(n, l, n))| = n + l - 1$, by the assumption that X_1', X_2' partition $\text{Lnodes}(G'(n, l, n))$ it must also be the case that $|X_1'|, |X_2'| < n$. We now show that both U_1 and U_2 are subsets of injectable sets and are hence injectable.

The case for U_1 proceeds as follows. Since $A_1^{[n]} \in U_1$ and $L_1^{[n]}$ is a parent of $A_1^{[n]}$, it must be that $L_1^{[n]} \in X_1'$. Since X_1' is totally adjacent by assumption, the adjacency sequence $x'_1, \dots, x'_{|X_1'|}$ of X_1' must be of the form

$$x'_1, \dots, x'_{|X_1'|} = L_1^{[n-|X_1'|+1]}, \dots, L_1^{[n]}. \quad (\text{A47})$$

The visible node $A_1^{[n-|X_1'|+1]}$ is not in U_1 since $L_1^{[n-|X_1'|]}$ is a parent of $A_1^{[n-|X_1'|+1]}$ but is not in X_1' . However, all other parents of $A_1^{[n-|X_1'|+1]}$ are in X_1' , so then $\text{Anc}_{G'(n, l, n)}(U_1 \cup \{A_1^{[n-|X_1'|+1]}\}) = X_1' \cup \{L_1^{[n-|X_1'|]}\}$. Similarly, $A_1^{[n-|X_1'|+2]}$ is not in $U_1 \cup \{A_1^{[n-|X_1'|+1]}\}$ since $L_1^{[n-|X_1'|+1]}$ is a parent of $A_1^{[n-|X_1'|+2]}$ but is not in $X_1' \cup \{L_1^{[n-|X_1'|]}\}$, while all other parents of $A_1^{[n-|X_1'|+2]}$ are. So then $\text{Anc}_{G'(n, l, n)}(U_1 \cup \{A_1^{[n-|X_1'|+2]}, A_1^{[n-|X_1'|+1]}\}) = X_1' \cup \{L_1^{[n-|X_1'|+1]}, L_1^{[n-|X_1'|]}\}$. Proceeding in this fashion, we can define

$$W_1 := U_1 \cup \{A_1^{[l]}, \dots, A_1^{[n-|X_1'|+l-1]}\} \quad (\text{A48})$$

and observe that $\text{Anc}_{G'(n, l, n)}(W_1)$ has n elements and is totally adjacent (the adjacency sequence is $L_1^{[1]}, \dots, L_1^{[n]}$). Thus W_1 is injectable by Lemma A3.

The case for U_2 proceeds similarly. Since $A_1^{[1]} \in U_2$ and $L_2^{[n-l+2]}$ is a parent of $A_1^{[1]}$, it must be that $L_2^{[n-l+2]} \in X_2'$. Since X_2' is totally adjacent by assumption, the adjacency sequence $y'_1, \dots, y'_{|X_2'|}$ of X_2' must be of the form

$$y'_1, \dots, y'_{|X_2'|} = L_2^{[n-l+2]}, \dots, L_2^{[n]}, L_1^{[1]}, \dots, L_1^{[|X_2'|-l+1]} \quad (\text{A49})$$

The visible node $A_1^{[X'_2|-l+2]}$ cannot be in U'_2 since $L_1^{[X'_2|-l+2]}$ is a parent of $A_1^{[X'_2|-l+2]}$ but is not in X'_2 . However, all other parents of $A_1^{[X'_2|-l+2]}$ are in X'_2 , so it follows that $\text{Anc}_{G'(n,l,n)}(U'_2 \cup \{A_1^{[X'_2|-l+2]}\}) = X'_2 \cup \{L_1^{[X'_2|-l+2]}\}$. Just as with the case above, we continue appending visible nodes to U'_2 until we obtain a provably injectable set. Explicitly, we define $W'_2 := U'_2 \cup \{A_1^{[X'_2|-l+2]}, \dots, A_1^{[n-l+1]}\}$ and get that $\text{Anc}_{G'(n,l,n)}(W'_2) = \{L_2^{[n-l+2]}, \dots, L_2^{[n]}, L_1^{[1]}, \dots, L_1^{[n-l+1]}\}$ is of size n and totally adjacent (with adjacency sequence $L_2^{[n-l+2]}, \dots, L_2^{[n]}, L_1^{[1]}, \dots, L_1^{[n-l+1]}$). By Lemma A3, W'_2 is injectable. ■

Let us now turn to the proof of Theorem 2, which we restate here for convenience, with the minor change of replacing $G'(n, l, j)$ for a general $j \in \{1, \dots, n\}$ with $G'(n, l, n)$ pursuant to the comments made earlier:

Theorem A1. Let $k \in \mathbb{N}_{>1}$ be odd. If $n \geq (l-1)k$, then there exists a partition $\{\mathcal{S}_1, \dots, \mathcal{S}_k\}$ of $\text{Vnodes}(G'(n, l, n))$ such that, taking $V := \{\mathcal{S}_1, \dots, \mathcal{S}_k\}$, all elements of $2^V \setminus V$ are injectable or expressible in $G'(n, l, n)$.

Proof of Theorem 2. Consider $G'(n, l, n)$ for $n \geq (l-1)k$ for some odd $k \in \mathbb{N}_{>1}$ and consider $\text{Lnodes}(G'(n, l, n))$ equipped with the order as in Eq. (A44).

Define $U'(r) := \{A_1^{[r]}, \dots, A_1^{[n-l+r]}\}$ for $r \in \{1, \dots, l\}$. Then,

$$\text{Anc}_{G'(n,l,n)}(U'(r)) = \begin{cases} \{L_2^{[n-l+1+r]}, \dots, L_2^{[n]}, L_1^{[1]}, \dots, L_1^{[n-l+r]}\}, & \text{if } r \in \{1, \dots, l-1\}, \\ \{L_1^{[1]}, \dots, L_1^{[n]}\}, & \text{if } r = l. \end{cases} \quad (\text{A50})$$

In either case, $\text{Anc}_{G'(n,l,n)}(U'(r))$ satisfies the conditions of Lemma A3 and hence $U'(r)$ is injectable.

Now define $U'_1(t) := \{A_1^{[n-t+1]}, A_1^{[n-t+2]}, \dots, A_1^{[n]}\}$ and $U'_2(t') = \{A_1^{[1]}, A_1^{[2]}, \dots, A_1^{[t']}\}$ for $t, t' \in \{1, \dots, n-l\}$. We get that

$$\text{Anc}_{G'(n,l,n)}(U'_1(t)) = \{L_1^{[n-l+2-t]}, \dots, L_1^{[n]}\}, \quad (\text{A51})$$

$$\text{Anc}_{G'(n,l,n)}(U'_2(t')) = \{L_2^{[n-l+2]}, \dots, L_2^{[n]}, L_1^{[1]}, \dots, L_1^{[t']}\}, \quad (\text{A52})$$

both of which are totally adjacent with respect to Eq. (A44). If in addition $t+t' = n-l+1$, then $\text{Anc}_{G'(n,l,n)}(U'_1(t))$ and $\text{Anc}_{G'(n,l,n)}(U'_2(t'))$ partition $\text{Lnodes}(G'(n, l, n))$, in which case $U'_1(t) \cup U'_2(t')$ is expressible.

Let us now define, for $r \in \{1, \dots, l\}$,

$$\mathcal{A}(r) := \begin{cases} \{A_1^{[1]}, \dots, A_1^{[l-1]}\}, & \text{if } r = l, \\ \{A_1^{[n-l+2]}, \dots, A_1^{[n]}\}, & \text{if } r = 1, \\ \{A_1^{[1]}, \dots, A_1^{[r-1]}\} \cup \{A_1^{[n-l+r+1]}, \dots, A_1^{[n]}\}, & \text{if } 1 < r < l, \end{cases} \quad (\text{A53})$$

and, for $t \in \{1, \dots, n-l\}$,

$$\mathcal{B}(t) := \{A_1^{[n-l+2-t]}, \dots, A_1^{[n-l]}\}. \quad (\text{A54})$$

Note that, for any r and t in the allowed ranges, $|\mathcal{A}(r)| = |\mathcal{B}(t)| = l-1$. Furthermore, we get that

$$\text{Vnodes}(G'(n, l, n)) \setminus \mathcal{A}(r) = U'(r), \quad (\text{A55})$$

$$\text{Vnodes}(G'(n, l, n)) \setminus \mathcal{B}(t) = U'_1(t) \cup U'_2(n-l+1-t), \quad (\text{A56})$$

so if we are able to construct a set partition of $\text{Vnodes}(G'(n, l, n))$ out of $\mathcal{A}(r)$, $\mathcal{B}(t)$ or sets containing

them for suitable values for r, t , then we are guaranteed that their set complements are injectable or expressible.

Since a set partition is made up of mutually disjoint sets, let us consider the conditions under which the $\mathcal{A}(r)$ and $\mathcal{B}(t)$ are disjoint. The sets $\mathcal{A}(r_1)$ and $\mathcal{A}(r_2)$ satisfy $\mathcal{A}(r_1) \cap \mathcal{A}(r_2) = \emptyset$ if $r_1 = 1$ and $r_2 = l$. The sets $\mathcal{B}(t_1)$ and $\mathcal{B}(t_2)$ satisfy $\mathcal{B}(t_1) \cap \mathcal{B}(t_2) = \emptyset$ if $|t_1 - t_2| > l-2$. The sets $\mathcal{A}(r)$ and $\mathcal{B}(t)$ satisfy $\mathcal{A}(r) \cap \mathcal{B}(t) = \emptyset$ if $r = 1$ and $t > l-2$, if $r = l$ and $t < n-2l+3$, or if $r \neq 1, l$ and $l-1 < t+r < n-l+3$.

Let us now define $\widehat{\mathcal{S}}_1 := \mathcal{A}(1)$ and $\widehat{\mathcal{S}}_q := \mathcal{B}((q-1)(l-1))$ for $q \in \{2, \dots, \kappa\}$ where $\kappa := 1 + \lfloor ((n-2l+3)/(l-1)) \rfloor$. To see that κ is well-defined (i.e., $\kappa \geq 2$), we

note that by assumption $n \geq k(l-1)$ and $l-1 > 0$, so

$$\frac{n-2l+3}{l-1} \geq \frac{k(l-1)-2l+3}{l-1} \geq k-2 + \frac{1}{l-1} \geq 1, \quad (\text{A57})$$

since k is both odd and greater than 1. In fact, the above reasoning demonstrates that $\kappa \geq k-1$. Note that the definitions of the $\widehat{\mathcal{S}}_i$ so far ensure that they are mutually disjoint: $\widehat{\mathcal{S}}_1 \cap \widehat{\mathcal{S}}_q = \emptyset$ since $(q-1)(l-1) \geq l-2$ for all $q \in \{2, \dots, \kappa\}$ and $\widehat{\mathcal{S}}_{q_1} \cap \widehat{\mathcal{S}}_{q_2} = \emptyset$ for all $q_1 \neq q_2 \in \{1, \dots, \kappa\}$ since $|(q_1-1)(l-1) - (q_2-1)(l-1)| = |(q_1-q_2)(l-1)| > l-2$. Furthermore, we have that

$$\bigcup_{i=1}^{\kappa} \widehat{\mathcal{S}}_i = \{A_1^{[n-\kappa(l-1)+1]}, \dots, A_1^{[n]}\}. \quad (\text{A58})$$

Let us then define $\widehat{\mathcal{S}}_{\kappa+1} := \{A_1^{[1]}, \dots, A_1^{[n-\kappa(l-1)]}\}$. As it stands, $\{\widehat{\mathcal{S}}_1, \dots, \widehat{\mathcal{S}}_{\kappa+1}\}$ forms a valid set partition of $\text{Vnodes}(G'(n, l, n))$. Furthermore, we know that $\text{Vnodes}(G'(n, l, n)) \setminus \widehat{\mathcal{S}}_q$ is injectable or expressible for each $q \in \{1, \dots, \kappa\}$ since

$$\text{Vnodes}(G'(n, l, n)) \setminus \widehat{\mathcal{S}}_1 = \mathcal{U}'(1) \quad (\text{A59})$$

and

$$\begin{aligned} \text{Vnodes}(G'(n, l, n)) \setminus \widehat{\mathcal{S}}_q &= \mathcal{U}'_1((q-1)(l-1)) \\ &\cup \mathcal{U}'_2(n - q(l-1)), \quad q \in \{2, \dots, \kappa\} \end{aligned} \quad (\text{A60})$$

by construction. To see that $\text{Vnodes}(G'(n, l, n)) \setminus \widehat{\mathcal{S}}_{\kappa+1}$ is injectable also, we note that

$$n - \kappa[l-1] \geq n - \frac{n-2l+3}{l-1}(l-1) \geq 2l-3 \geq l-1, \quad (\text{A61})$$

where the last inequality uses that $l \geq 2$. In particular, this means that $\widehat{\mathcal{S}}_{\kappa+1} \supseteq \mathcal{A}(l)$ and hence that $\text{Vnodes}(G'(n, l, n)) \setminus \widehat{\mathcal{S}}_{\kappa+1} \subseteq \mathcal{U}'(l)$, from which injectability follows (recall that subsets of injectable sets are injectable).

Finally, it remains only to construct a partition using precisely k subsets. From above, we know that $\kappa \geq k-1$ meaning that $\kappa+1 \geq k$, so the partition $\{\widehat{\mathcal{S}}_1, \dots, \widehat{\mathcal{S}}_{\kappa+1}\}$ has at least as many elements as required. If $\kappa+1 = k$, taking $\mathcal{S}_q = \widehat{\mathcal{S}}_q$ for all $q \in \{1, \dots, \kappa+1\}$ finishes the job. In the case where $\kappa+1 > k$, we can simply define a partition $\{\mathcal{S}_1, \dots, \mathcal{S}_k\}$ where one or more of the $\mathcal{S}_i$ consist of a union of $\widehat{\mathcal{S}}_q$. For example, by taking $\mathcal{S}_q = \widehat{\mathcal{S}}_q$ for all $q = 1, \dots, k-1$ and $\mathcal{S}_k := \bigcup_{i=k}^{\kappa+1} \widehat{\mathcal{S}}_i$. In this case, $\text{Vnodes}(G'(n, l, n)) \setminus \mathcal{S}_q \subseteq \text{Vnodes}(G'(n, l, n)) \setminus \widehat{\mathcal{S}}_q$ for all $q \in \{1, \dots, k\}$ and so remain injectable or expressible.

Thus, for $\mathbf{V} := \{\mathcal{S}_1, \dots, \mathcal{S}_k\}$, each element of $2^{\mathbf{V}} \setminus \mathbf{V}$ is injectable or expressible as required. ■

Using Lemmas A3 and A4, we can now justify the claims made in Sec. VI regarding the injectable and expressible sets of the pentagon and woven hexagon scenarios. For the Cut inflation $G'(5, 2, 5)$ of the pentagon scenario $G(5, 2)$, we consider $\text{LNodes}(G'(5, 2, 5))$ with the order

$$L_2^{[5]} < L_1^{[1]} < L_1^{[2]} < L_1^{[3]} < L_1^{[4]} < L_1^{[5]}. \quad (\text{A62})$$

For $\mathcal{U}' := \{A_1^{[1]}, A_1^{[2]}, A_1^{[3]}, A_1^{[4]}\}$, we have that

$$\begin{aligned} \text{Anc}_{G'(5,2,5)}(\{A_1^{[1]}, A_1^{[2]}, A_1^{[3]}, A_1^{[4]}\}) \\ = \{L_2^{[5]}, L_1^{[1]}, L_1^{[2]}, L_1^{[3]}, L_1^{[4]}\} \end{aligned} \quad (\text{A63})$$

which has five elements and is totally adjacent with adjacency sequence $L_2^{[5]}, L_1^{[1]}, L_1^{[2]}, L_1^{[3]}, L_1^{[4]}$, so by Lemma A3, $\mathcal{U}'$ is injectable. For $\mathcal{U}' := \{A_1^{[2]}, A_1^{[3]}, A_1^{[4]}, A_1^{[5]}\}$, we have that

$$\begin{aligned} \text{Anc}_{G'(5,2,5)}(\{A_1^{[2]}, A_1^{[3]}, A_1^{[4]}, A_1^{[5]}\}) \\ = \{L_1^{[1]}, L_1^{[2]}, L_1^{[3]}, L_1^{[4]}, L_1^{[5]}\}, \end{aligned} \quad (\text{A64})$$

which also has 5 elements and is totally adjacent (with adjacency sequence $L_1^{[1]}, L_1^{[2]}, L_1^{[3]}, L_1^{[4]}, L_1^{[5]}$), so is injectable.

Defining $\mathcal{U}'_1 := \{A_1^{[1]}, A_1^{[2]}, A_1^{[3]}\}$ and $\mathcal{U}'_2 := \{A_1^{[5]}\}$, we get that

$$\begin{aligned} \text{Anc}_{G'(5,2,5)}(\{A_1^{[1]}, A_1^{[2]}, A_1^{[3]}\}) &= \{L_2^{[5]}, L_1^{[1]}, L_1^{[2]}, L_1^{[3]}\}, \\ \text{Anc}_{G'(5,2,5)}(\{A_1^{[5]}\}) &= \{L_1^{[4]}, L_1^{[5]}\}, \end{aligned} \quad (\text{A65})$$

both of which are totally adjacent with respect to the order in Eq. (A62) and which form a partition of $\text{LNodes}(G'(5, 2, 5))$. So by Lemma A4, $\{A_1^{[1]}, A_1^{[2]}, A_1^{[3]}, A_1^{[5]}\}$ is expressible. The cases where $\mathcal{U}'_1 := \{A_1^{[1]}, A_1^{[2]}\}$ and $\mathcal{U}'_2 = \{A_1^{[4]}, A_1^{[5]}\}$, and where $\mathcal{U}'_1 := \{A_1^{[1]}\}$ and $\mathcal{U}'_2 = \{A_1^{[3]}, A_1^{[4]}, A_1^{[5]}\}$, proceed analogously.

For the Cut inflation $G'(6, 3, 6)$ of the woven hexagon scenario $G(6, 3)$, we consider the order on $\text{LNodes}(G'(6, 3, 6))$ given by

$$L_2^{[5]} < L_2^{[6]} < L_1^{[1]} < L_1^{[2]} < L_1^{[3]} < L_1^{[4]} < L_1^{[5]} < L_1^{[6]}. \quad (\text{A66})$$

Analogously to the pentagon scenario, Lemma A3 can be used to show that $\{A_1^{[1]}, A_1^{[2]}, A_1^{[3]}, A_1^{[4]}\}$, $\{A_1^{[2]}, A_1^{[3]}, A_1^{[4]}, A_1^{[5]}\}$, and $\{A_1^{[3]}, A_1^{[4]}, A_1^{[5]}, A_1^{[6]}\}$ are injectable, and Lemma A4 can be used to show that $\{A_1^{[1]}, A_1^{[2]}, A_1^{[3]}\} \cup \{A_1^{[6]}\}$, $\{A_1^{[1]}, A_1^{[2]}\} \cup \{A_1^{[5]}, A_1^{[6]}\}$, and $\{A_1^{[1]}\} \cup \{A_1^{[4]}, A_1^{[5]}, A_1^{[6]}\}$ are expressible.

APPENDIX B: HIGHER-DIMENSIONAL GENERALIZED SCHMIDT DECOMPOSITION

The following is a summary of the generalized Schmidt decomposition presented in [Thm 2, 58]. After presenting the general case, we consider the specific case considered in Sec. V.

Consider $\mathcal{H} = \bigotimes_{i=1}^n \mathcal{H}_i$ with $n \geq 3$ and let $d_i := \dim \mathcal{H}_i$ and $D := \dim \mathcal{H}$. Let us label the component Hilbert

spaces such that $2 \leq d_1 \leq \dots \leq d_n$. Let $\{I_1, \dots, I_N\}$ be the ordered set of length $(n-1)$ tuples $(i_1, \dots, i_{n-1})$ with $1 \leq i \leq d_k$ which excludes tuples of the form $(i, \dots, i)$ and $(d_1, \dots, d_k, i, \dots, i)$ with $d_k \leq i < d_{k+1}$ and $1 \leq k \leq n-2$. The ordering of $\{I_1, \dots, I_N\}$ is lexicographical. Define the set $\mathcal{B}_0$ to be the set of n -tuples $(i_1, \dots, i_n)$ with $(i_1, \dots, i_{n-1}) = I_k$ and $i_n = d_{n-1} + l$ where $1 \leq k \leq \min\{N, d_n - d_{n-1}\}$ and $k \leq l \leq d_n - d_{n-1}$. Define also the following sets of n -tuples:

$$\mathcal{B}_1 := \{(d_1, \dots, d_{k-1}, j, d_{k+1}, \dots, d_{n-1}, d_{n-1}) : 1 \leq j < d_k, 1 \leq k \leq n-2\} \quad (\text{B1})$$

$$\mathcal{B}_2 := \{(d_1, \dots, d_{n-2}, j, d_{n-1}) : 1 \leq j < d_{n-2}\}, \quad (\text{B2})$$

$$\mathcal{B}_3 := \{(d_1, \dots, d_{n-2}, j, 1) : d_{n-2} \leq j \leq d_{n-1}\}, \quad (\text{B3})$$

$$\mathcal{B}_4 := \{(j, j, \dots, j) : 2 \leq j \leq d_1\} \cup \{(d_1, \dots, d_k, j, \dots, j) : 1 \leq k < n-1, d_k < j \leq d_{k+1}\} \\ \cup \left\{ (d_1, \dots, d_{n-1}, j) : d_{n-1} < j \leq \min \left\{ \frac{D}{d_n}, d_n \right\} \right\}. \quad (\text{B4})$$

Any $|\Psi\rangle \in \mathcal{H}$ can be written as

$$|\Psi\rangle = \sum_{i_1, \dots, i_n} \alpha_{i_1 \dots i_n} |\psi_{i_1}^{(1)} \dots \psi_{i_n}^{(n)}\rangle, \quad (\text{B5})$$

where $\{|\psi_j\rangle^{(k)}\}_{j=1}^{d_k}$ is a basis for $\mathcal{H}_k$ for each k and where the coefficients $\alpha_{i_1 \dots i_n}$ satisfy

- (1) $\alpha_{ii \dots ijii \dots i} = 0$ if $1 \leq i < d_1$ and $i < j$,
- (2) $\alpha_{d_1 \dots d_k ii \dots ijii \dots i} = 0$ if $d_k \leq i < d_{k+1}$ and $i < j$, $1 \leq k \leq n-2$,
- (3) α_I for every n -tuple index $I \in \mathcal{B}_0$,
- (4) the coefficients with indices in the sets $\mathcal{B}_x$, $x = 1, \dots, 4$ are real and non-negative,
- (5) for $i = 1, \dots, d_{n-1}$, define

$$R_i = |\alpha_{d_1 \dots d_k i \dots i}|, \quad (\text{B6})$$

where k is such that $d_k < i \leq d_{k+1}$. Then $R_1 \geq \dots \geq R_{d_{n-1}}$.

In Sec. V, we consider pure-states in $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C \cong \mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathbb{C}^4$. This means that $d_1 = d_2 = 2$, $d_3 = 4$, $D = 16$, and $N = 3$. We have that

$$\{I_1, I_2, I_3\} = \{(1, 2), (2, 1), (2, 2)\}, \quad (\text{B7})$$

$$\mathcal{B}_0 = \{(1, 2, 3), (1, 2, 4), (2, 1, 4)\}, \quad (\text{B8})$$

$$\mathcal{B}_1 = \{(1, 2, 2)\}, \quad (\text{B9})$$

$$\mathcal{B}_2 = \{(2, 1, 2)\}, \quad (\text{B10})$$

$$\mathcal{B}_3 = \{(2, 2, 1)\}, \quad (\text{B11})$$

$$\mathcal{B}_4 = \{(2, 2, 2)\} \cup \emptyset \cup \{(2, 2, 3), (2, 2, 4)\}. \quad (\text{B12})$$

From item (1), we get that $\alpha_{112} = \alpha_{121} = \alpha_{211} = \alpha_{113} = \alpha_{114} = 0$. Item (2) does not rule out any coefficients. Item (3) ensures that $\alpha_{123} = \alpha_{124} = \alpha_{214} = 0$. Item (4) gives that $\alpha_{122}, \alpha_{212}, \alpha_{221}, \alpha_{222}, \alpha_{223}, \alpha_{224} \in \mathbb{R}_{\geq 0}$, and item (5) requires that $|\alpha_{111}| \geq |\alpha_{222}|$.

To arrive at the form given in Eq. (72), we make a few notational modifications. First, we identify the bases $\{|\psi_j\rangle^{(k)}\}_{j=1}^{d_k}$ for $k = A, B, C$ with the computational basis in each case (i.e., $\{|0\rangle, |1\rangle\}$ for A and B , and $\{|0\rangle, \dots, |3\rangle\}$ for C). We write each coefficient not constrained to be real and positive in polar form and relabel all nonzero coefficients α_{ijk} to α_x for $x = 0, \dots, 7$ where the ordering corresponds to the lexicographical ordering of the corresponding computational basis states.

APPENDIX C: SOME INFLATIONS PRODUCE TRIVIAL WITNESSES

For the networks considered throughout this paper, we focused on a single type of nonfanout inflation, namely that of the Cut inflation. However, for a given network G , various choices of nonfanout inflation are often available. It is then natural to ask whether these other choices also lead to nontrivial G -incompatibility witnesses. Here, we demonstrate that this is not guaranteed to be the case.

Consider the nonfanout inflation of the triangle scenario depicted in Fig. 5, which is known as the Ring inflation

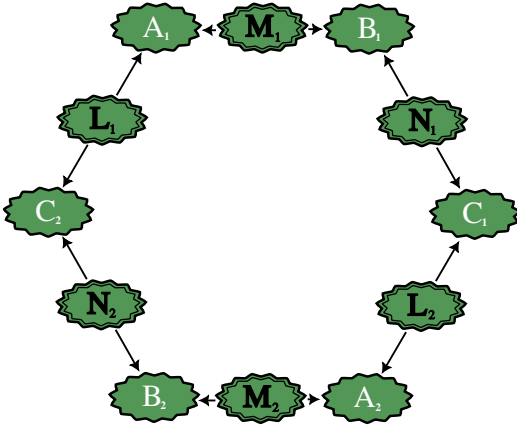


FIG. 5. The Ring inflation of the triangle scenario. Note that, despite the similar structure, this directed acyclic graph is distinct from that of the network $G(6, 2)$ from the family of networks considered in Sec. VI, as it is an inflation of the triangle scenario and hence has node labels that are the same up to copy-indices as those of the triangle scenario [i.e., the network $G(3, 2)$].

[22,86]. For this inflation, the sets

$$\begin{aligned} \{A_1, B_1\}, \quad \{B_1, C_1\}, \quad \{C_1, A_2\}, \quad \{A_2, B_2\}, \\ \{B_2, C_2\}, \quad \{C_2, A_2\} \end{aligned} \quad (C1)$$

are all injectable. Furthermore, any pair of sets that differ only in their copy-indices — $\{A_1, B_1\}$ and $\{A_2, B_2\}$, for example — share no common ancestors, meaning that

$$\{A_1, B_1, A_2, B_2\}, \quad \{A_1, C_1, A_2, C_2\}, \quad \{B_1, C_1, B_2, C_2\} \quad (C2)$$

and all subsets thereof are expressible.

Let $\mathbf{V} := \{S_1, S_2, S_3\}$ with $S_1 := \{A_1, A_2\}$, $S_2 := \{B_1, B_2\}$ and $S_3 := \{C_1, C_2\}$. The set $\mathbf{V}$ defines a partition of the visible nodes of the Ring inflation and moreover, $2^{\mathbf{V}} \setminus \mathbf{V}$ consists of injectable and expressible sets as established above. As per Sec. VI, we are thus in a position to write down a candidate triangle-incompatibility witness based on the inequality from Hall [cf. Eq. (30)]. For ρ_{ABC} a state on the Hilbert spaces associated with the visible nodes of the triangle scenario, the triangle-incompatibility witness for the choice of $\mathbf{V}$ defined above is

$$\begin{aligned} I^{\text{Ring}}(\rho_{ABC}) = \mathbb{1} - \rho_A \otimes \rho_A - \rho_B \otimes \rho_B - \rho_C \otimes \rho_C \\ + \rho_{AB} \otimes \rho_{AB} + \rho_{AC} \otimes \rho_{AC} + \rho_{BC} \otimes \rho_{BC}, \end{aligned} \quad (C3)$$

where each term in the above expression is to be understood as an operator on $\mathcal{H}_{A_1} \otimes \mathcal{H}_{B_1} \otimes \mathcal{H}_{C_1} \otimes \mathcal{H}_{A_2} \otimes \mathcal{H}_{B_2} \otimes \mathcal{H}_{C_2}$ (that is, the identity operators have again been omitted from the notation as has been done throughout this paper).

Despite being expressed entirely in terms of marginals of ρ_{ABC} , just like the triangle-incompatibility witnesses derived from the Cut inflation, I^{Ring} is a trivial triangle-incompatibility witness. That is, $I^{\text{Ring}}(\rho_{ABC})$ is positive semidefinite for all ρ_{ABC} , meaning that the triangle-incompatibility of no state ρ_{ABC} can be witnessed. To see that $I^{\text{Ring}}(\rho_{ABC})$ is positive semidefinite, let us define $\mathcal{H}_A := \mathcal{H}_{A_1} \otimes \mathcal{H}_{A_2}$ and similarly for $\mathcal{H}_B$ and $\mathcal{H}_C$. Let σ be a state on $\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C$ given by $\sigma = \rho_{ABC} \otimes \rho_{ABC}$, with the ordering of the Hilbert spaces such that the two copies of ρ_{ABC} corresponding to $\mathcal{H}_{A_1} \otimes \mathcal{H}_{B_1} \otimes \mathcal{H}_{C_1}$ and $\mathcal{H}_{A_2} \otimes \mathcal{H}_{B_2} \otimes \mathcal{H}_{C_2}$ respectively. For $\mathbf{V}' := \{A, B, C\}$, Eq. (30) guarantees that

$$\Delta(\{\sigma_{\mathbf{X}} : \mathbf{X} \in 2^{\mathbf{V}'} \setminus \mathbf{V}'\}) \geq 0. \quad (C4)$$

However, $\Delta(\{\sigma_{\mathbf{X}} : \mathbf{X} \in 2^{\mathbf{V}'} \setminus \mathbf{V}'\})$ is precisely the operator $I^{\text{Ring}}(\rho_{ABC})$,

$$\begin{aligned} \Delta(\{\sigma_{\mathbf{X}} : \mathbf{X} \in 2^{\mathbf{V}'} \setminus \mathbf{V}'\}) \\ = \mathbb{1} - \sigma_A - \sigma_B - \sigma_C + \sigma_{AB} + \sigma_{AC} + \sigma_{BC} \end{aligned} \quad (C5)$$

$$\begin{aligned} = \mathbb{1} - \rho_A \otimes \rho_A - \rho_B \otimes \rho_B - \rho_C \otimes \rho_C + \rho_{AB} \otimes \rho_{AB} \\ + \rho_{AC} \otimes \rho_{AC} + \rho_{BC} \otimes \rho_{BC} \end{aligned} \quad (C6)$$

$$= I^{\text{Ring}}(\rho_{ABC}). \quad (C7)$$

This example indicates that some care needs to be taken when leveraging the inequality of Eq. (30) in the pursuit of nontrivial G -incompatibility witnesses for a given network scenario G . An analysis of the conditions under which a nontrivial witness can be derived is left for future work.

APPENDIX D: EXAMPLE ILLUSTRATING PROPOSITION 1

In this appendix, we provide an example that illustrates the content of Proposition 1, which we have restated here:

Proposition D1. Let G' be an inflation of the network G . In this case, if the family of states $\{\rho_U : U \in \text{ImagesInjectableSets}(G)\}$ is compatible with G , then the family of states $\{\sigma_{Y'} : Y' \in \text{ExpressibleSets}(G')\}$, where

$$\sigma_{Y'} := \bigotimes_{U \in \text{ImagesInjectableComponents}(Y')} \rho_U \quad (D1)$$

is compatible with G' .

In our example, let G be the triangle scenario and let G' be the AB -Cut inflation of G . Recall that the singleton sets $\{A_1\}$, $\{B_1\}$, and $\{C_1\}$ are all injectable sets by the definition of inflation and hence are elements of $\text{ExpressibleSets}(G')$. Similarly, the sets $\{A_1, C_1\}$ and $\{B_1, C_1\}$ are also injectable in the AB -Cut inflation of the triangle, while $\{A_1, B_1\}$ is not injectable but is expressible, with injectable components given by $\{A_1\}$ and $\{B_1\}$.

Suppose that $\{\rho_U : U \in \text{ImagesInjectableSets}(G)\}$ is compatible with G . In particular, this means that there exists a state ρ_{ABC} and a set of parameters

$$\text{par} := \{\mathcal{E}_{A|L^{(A)}M^{(A)}}, \mathcal{E}_{B|M^{(B)}N^{(B)}}, \mathcal{E}_{C|L^{(C)}N^{(C)}}, \rho_L, \rho_M, \rho_N\}, \quad (\text{D2})$$

where the maps $\mathcal{E}_{A|L^{(A)}M^{(A)}}$, $\mathcal{E}_{B|M^{(B)}N^{(B)}}$, $\mathcal{E}_{C|L^{(C)}N^{(C)}}$ and states $\rho_L = \rho_{L^{(A)}L^{(C)}}$, $\rho_M = \rho_{M^{(A)}M^{(B)}}$, $\rho_N = \rho_{N^{(B)}N^{(C)}}$ are as in Sec. II B, such that

$$\rho_{ABC} = \mathcal{E}_{A|L^{(A)}M^{(A)}} \otimes \mathcal{E}_{B|M^{(B)}N^{(B)}} \otimes \mathcal{E}_{C|L^{(C)}N^{(C)}} (\rho_{L^{(A)}L^{(C)}} \otimes \rho_{M^{(A)}M^{(B)}} \otimes \rho_{N^{(B)}N^{(C)}}). \quad (\text{D3})$$

Let us now consider the set of parameters par' given by $\text{par}' = \text{Inflation}_{G \rightarrow G'}(\text{par})$. That is, we consider the latent spaces of G' to be given by $\mathcal{H}_{L_1} \cong \mathcal{H}_L$, $\mathcal{H}_{M_1} \cong \mathcal{H}_{M^{(B)}}$, $\mathcal{H}_{M_2} \cong \mathcal{H}_{M^{(A)}}$ and $\mathcal{H}_{N_1} \cong \mathcal{H}_N$ and the visible space to be $\mathcal{H}_{A_1} \cong \mathcal{H}_A$, $\mathcal{H}_{B_1} \cong \mathcal{H}_B$ and $\mathcal{H}_{C_1} \cong \mathcal{H}_C$. The set par' is then

$$\text{par}' = \{\mathcal{E}_{A_1|L_1^{(A_1)}M_2}, \mathcal{E}_{B_1|M_1N_1^{(B_1)}}, \mathcal{E}_{C_1|L_1^{(C_1)}N_1^{(C_1)}}, \rho_{L_1}, \rho_{M_1}, \rho_{M_2}, \rho_{N_1}\}, \quad (\text{D4})$$

where

$$\mathcal{E}_{A_1|L_1^{(A_1)}M_2} \equiv \mathcal{E}_{A|L^{(A)}M^{(A)}}, \quad \mathcal{E}_{B_1|M_1N_1^{(B_1)}} \equiv \mathcal{E}_{B|M^{(B)}N^{(B)}}, \quad \mathcal{E}_{C_1|L_1^{(C_1)}N_1^{(C_1)}} \equiv \mathcal{E}_{C|L^{(C)}N^{(C)}}, \quad (\text{D5})$$

$$\rho_{L_1} \equiv \rho_{L^{(A)}L^{(C)}}, \quad \rho_{M_1} \equiv \rho_{M^{(B)}}, \quad \rho_{M_2} \equiv \rho_{M^{(A)}}, \quad \rho_{N_1} \equiv \rho_{N^{(B)}N^{(C)}}, \quad (\text{D6})$$

with “ $\equiv$ ” denoting equality up to the substitution of isomorphic Hilbert spaces (i.e., $\mathcal{E}_{A|L^{(A)}M^{(A)}}$ is a map from $\mathcal{H}_{L^{(A)}} \otimes \mathcal{H}_{M^{(A)}}$ to $\mathcal{H}_A$ where as $\mathcal{E}_{A_1|L_1^{(A_1)}M_2}$ is a map from $\mathcal{H}_{L_1^{(A_1)}} \otimes \mathcal{H}_{M_2} \cong \mathcal{H}_{L^{(A)}} \otimes \mathcal{H}_{M^{(A)}}$ to $\mathcal{H}_{A_1} \cong \mathcal{H}_A$, and similarly for the other parameters). Consequently, we can consider the state $\sigma_{A_1B_1C_1} \in \mathcal{L}(\mathcal{H}_{A_1} \otimes \mathcal{H}_{B_1} \otimes \mathcal{H}_{C_1})$ is given by

$$\sigma_{A_1B_1C_1} := \mathcal{E}_{A_1|L_1^{(A_1)}M_2} \otimes \mathcal{E}_{B_1|M_1N_1^{(B_1)}} \otimes \mathcal{E}_{C_1|L_1^{(C_1)}N_1^{(C_1)}} (\rho_{L_1} \otimes \rho_{M_1} \otimes \rho_{M_2} \otimes \rho_{N_1}). \quad (\text{D7})$$

If we consider the marginals of $\sigma_{A_1B_1C_1}$, we see that

$$\sigma_{A_1} = \text{Tr}_{B_1C_1} [\mathcal{E}_{A_1|L_1^{(A_1)}M_2} \otimes \mathcal{E}_{B_1|M_1N_1^{(B_1)}} \otimes \mathcal{E}_{C_1|L_1^{(C_1)}N_1^{(C_1)}} (\rho_{L_1} \otimes \rho_{M_1} \otimes \rho_{M_2} \otimes \rho_{N_1})] \quad (\text{D8})$$

$$= \mathcal{E}_{A_1|L_1^{(A_1)}M_2} (\rho_{L_1^{(A_1)}} \otimes \rho_{M_2}) \quad (\text{D9})$$

$$\equiv \mathcal{E}_{A|L^{(A)}M^{(A)}} (\rho_{L^{(A)}} \otimes \rho_{M^{(A)}}) \quad (\text{D10})$$

$$= \rho_A \quad (\text{D11})$$

and similarly for the marginals σ_{B_1} and σ_{C_1} . Likewise,

$$\sigma_{A_1C_1} = \text{Tr}_{B_1} [\mathcal{E}_{A_1|L_1^{(A_1)}M_2} \otimes \mathcal{E}_{B_1|M_1N_1^{(B_1)}} \otimes \mathcal{E}_{C_1|L_1^{(C_1)}N_1^{(C_1)}} (\rho_{L_1} \otimes \rho_{M_1} \otimes \rho_{M_2} \otimes \rho_{N_1})] \quad (\text{D12})$$

$$= \mathcal{E}_{A_1|L_1^{(A_1)}M_2} \otimes \mathcal{E}_{C_1|L_1^{(C_1)}N_1^{(C_1)}} (\rho_{L_1} \otimes \rho_{M_2} \otimes \rho_{N_1^{(C_1)}}) \quad (\text{D13})$$

$$\equiv \mathcal{E}_{A|L^{(A)}M^{(A)}} \otimes \mathcal{E}_{C|L^{(C)}N^{(C)}} (\rho_L \otimes \rho_{M^{(A)}} \otimes \rho_{N^{(C)}}) \quad (\text{D14})$$

$$= \rho_{AC} \quad (\text{D15})$$

and similarly for $\sigma_{B_1C_1}$. In the case of $\sigma_{A_1B_1}$, we get that

$$\sigma_{A_1B_1} = \text{Tr}_{C_1} [\mathcal{E}_{A_1|L_1^{(A_1)}M_2} \otimes \mathcal{E}_{B_1|M_1N_1^{(B_1)}} \otimes \mathcal{E}_{C_1|L_1^{(C_1)}N_1^{(C_1)}} (\rho_{L_1} \otimes \rho_{M_1} \otimes \rho_{M_2} \otimes \rho_{N_1})] \quad (\text{D16})$$

$$= \mathcal{E}_{A_1|L_1^{(A_1)}M_2} \otimes \mathcal{E}_{B_1|M_1N_1^{(B_1)}} (\rho_{L_1^{(A_1)}} \otimes \rho_{M_1} \otimes \rho_{M_2} \otimes \rho_{N_1^{(B_1)}}) \quad (\text{D17})$$

$$= \mathcal{E}_{A_1|L_1^{(A_1)}M_2} (\rho_{L_1^{(A_1)}} \otimes \rho_{M_1}) \otimes \mathcal{E}_{B_1|M_1N_1^{(B_1)}} (\rho_{M_1} \otimes \rho_{N_1^{(B_1)}}) \quad (\text{D18})$$

$$\equiv \rho_A \otimes \rho_B. \quad (\text{D19})$$

Since the states $\sigma_{A_1} \equiv \rho_A$, $\sigma_{B_1} \equiv \rho_B$, $\sigma_{C_1} \equiv \rho_C$, $\sigma_{A_1B_1} \equiv \rho_A \otimes \rho_B$, $\sigma_{A_1C_1} \equiv \rho_{AC}$, and $\sigma_{B_1C_1} \equiv \rho_{BC}$ are all marginals of $\sigma_{A_1B_1C_1}$ which is compatible with G' , it follows that the set $\{\rho_A, \rho_B, \rho_C, \rho_A \otimes \rho_B, \rho_{AC}, \rho_{BC}\}$ is compatible with G' . Proposition 1 establishes this implication for general networks G and inflations G' thereof.

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- [24] When multipartite entanglement is studied within the framework of resource theories, one can make different choices for the free operations relative to which it is considered a resource [23]. We summarize the main distinctions here. If each party can implement any unitary operation in their local lab, then we refer to the free operations as *Local Unitaries* (LU). If they can implement any quantum operation, then we refer to the free operations as *Local Operations* (LO). If all parties have access to a common source of classical randomness (i.e., a dice roll or a coin flip) that produces an outcome which may influence the operation that each party implements, then we refer to the free operations as *Local Operations with Shared Randomness* (LOSR). If, in addition to this shared randomness, the parties have access to bipartite entangled quantum states distributed pairwise between parties, then we refer to the free operations as *Local Operations with Shared Randomness and 2-Way Shared Entanglement* (LOSR2WSE). If no shared randomness is available but pairwise entanglement is, then we refer to the free operations as LO2WSE and if the allowed operations are restricted to being unitary, then we refer to the free operations as LU2WSE. If the parties do not have access to pairwise entanglement but do have access to classical communication channels between them (which subsumes having access to shared randomness), then we refer to the free operations as *Local Operations and Classical Communication* (LOCC).
- [25] To see this, we suppose that one can prepare the pure-state $|\Psi\rangle_{ABC}$ using LOSR2WSE and show that it follows that one can also prepare it without making use of the shared randomness, i.e., with just LO2WSE. Suppose the shared randomness consists of sampling a variable Λ from a distribution P_Λ and that in the LOSR2WSE protocol, the state prepared for the value $\Lambda = \lambda$ is denoted $|\psi_\lambda\rangle_{ABC}$, such that the overall state prepared in the protocol is $\rho_{ABC} = \sum_\lambda P_\Lambda(\lambda) |\psi_\lambda\rangle\langle\psi_\lambda|_{ABC}$. By virtue of the convex extremality of the state $|\Psi\rangle_{ABC}$, the only way to have $\rho_{ABC} = |\Psi\rangle\langle\Psi|_{ABC}$ is if $|\psi_\lambda\rangle_{ABC} = |\Psi\rangle_{ABC}$ for all λ that are assigned nonzero probability by P_Λ . But this implies that the protocol allows for the preparation $|\Psi\rangle_{ABC}$ without use of the shared randomness.
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- [27] Reference [26] did not allow for tracing out subsystems, which is why the two approaches are distinct in spite of the Stinespring dilation theorem.
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- [29] There is no loss of generality in doing so in the case of classical causal modelling because Ref. [90] showed that every partitioned DAG is observationally equivalent to one wherein all the latent nodes are exogenous.
- [30] A comment regarding notation: if $\text{Pa}(A)$ is empty, then $P_{A|\text{Pa}(A)} = P_A$.
- [31] E. Wolfe, A. Pozas-Kerstjens, M. Grinberg, D. Rosset, A. Acín, and M. Navascués, Quantum inflation: A general approach to quantum causal compatibility, *Phys. Rev. X* **11**, 021043 (2021).
- [32] This terminology can also be motivated by recent developments of quantum networks within the context of the quantum internet [91,92]. For example, several proposals exist for satellite-based “downlink” quantum networks (see, e.g., Refs. [68,93]) whereby satellites act as sources distributing entangled states to separated receiver stations on the ground. In such cases, if the satellites are considered to be the latent nodes of the network and the ground stations the visible nodes, and if the lack of communication between these nodes can be justified on practical grounds (i.e., due to the separation of satellites in orbit or the stations on the ground [94]), then the topology of these downlink networks matches the type of causal structures termed networks here.
- [33] The assumption that the latent spaces are finite-dimensional derives from nuances regarding the definition of causal compatibility that occur if this assumption is dropped—see the comments below Definition 2.
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- [37] We note that the definition of a state being compatible with the triangle scenario using quantum latents, asks about the existence of arbitrary quantum channels $\mathcal{E}_{A|L^{(A)}M^{(A)}}, \mathcal{E}_{B|M^{(B)}N^{(B)}},$ and $\mathcal{E}_{C|L^{(C)}N^{(C)}}$ in Eq. (4). In Refs. [26,95], by contrast, these quantum channels are restricted to be unitary channels. Consequently, the notion of compatibility defined here is more permissive than the notion of compatibility proposed in Refs. [26,95]. Because we cannot see a good reason to restrict these channels to unitaries, we consider the notion of compatibility described above to be the fundamental one, rather than that of Refs. [26,95]. Nonetheless, there are cases where the two definitions coincide, such as when studying compatibility of pure-states. See Sec. IV A for a discussion of this case.
- [38] In particular, this means that $U'_{(j)}$ and $U'_{(k)}$ are d -separated by the empty set in G' . Also note that, in Ref. [15], a more general definition of expressible set was given, with the notion presented here being referred to as “ai-expressibility” (with “ai” standing for “ancestrally independent”). However, in the case where G is a network, the set of ai-expressible sets is equal to the set of all expressible sets. As we focus exclusively on networks in this article, we refrain from providing the full definition here.
- [39] Note that in Ref. [15], the pair consisting of G and a particular choice of parameter values, par , was referred to as a *causal model*. For physicists, the term “model” appears natural as the description of a *particular* choice of parameter values. For statisticians, however, the term “model” naturally corresponds to a *set* of possible such choices. To reduce confusion, we here use the term “causal model” in a manner that is more in keeping with the statistician’s usage.
- [40] The map $\text{Inflation}_{G \rightarrow G'}$ has been defined in this way since we focus on networks G in this work, meaning that no latent node of G has any parents. It should be noted, however, that there are DAGs G where latent nodes *do* have parents in G . To cover this more general case, the inflation map can be defined without distinguishing between latent and visible nodes as is done above: for each $X_i \in \text{Nodes}(G')$, $\text{Inflation}_{G \rightarrow G'}$ assigns to X_i the parameter $\mathcal{E}_{X_i|\tilde{\text{Pa}}_{G'}(X_i)} = \mathcal{E}_{X_i|\tilde{\text{Pa}}_G(X)}$ with the understanding that (a) if $\tilde{\text{Pa}}_{G'}(X_i)$ is empty, the map is a state-preparation and (b) if the children of X_i in G' is a subset of the set of children of X in G (up to sameness of copy-indices), then there is a partial trace over the unused subspaces of X_i to produce the reduced state on those subspaces corresponding to $\text{Ch}(X_i)$, as in (ii) above.
- [41] Equivalently, one can define an inflation as nonfanout if the *descendent subgraph* of every latent node in the inflation DAG is the same up to copy-indices as the *descendent subgraph* of the corresponding latent node in the original DAG.
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- [47] For pedagogical purposes, we here explain why there is a difference between the cases of even and odd numbers of

systems. In Ref. [19], it is shown that the operator

$$\Lambda(\{\sigma_{\mathbf{X}} : \mathbf{X} \in 2^{\mathbf{V}}\}) := \sum_{\mathbf{X} \in 2^{\mathbf{V}}} (-1)^{|\mathbf{X}|} \sigma_{\mathbf{X}} \otimes \mathbb{I}_{\mathbf{V} \setminus \mathbf{X}} \quad (32)$$

is positive for any cardinality of $\mathbf{V}$. However, this is not the same as Eq. (31) being positive for any cardinality of $\mathbf{V}$, since the sum in the above expression includes the case where $\mathbf{X} = \mathbf{V}$ while the sum in Eq. (31) does not. For odd cardinality of $\mathbf{V}$, we have that

$$\Lambda(\{\sigma_{\mathbf{X}} : \mathbf{X} \in 2^{\mathbf{V}}\}) = \Lambda(\{\sigma_{\mathbf{X}} : \mathbf{X} \in 2^{\mathbf{V}} \setminus \mathbf{V}\}) - \sigma_{\mathbf{V}}, \quad (33)$$

while for even cardinality of $\mathbf{V}$, we have

$$\Lambda(\{\sigma_{\mathbf{X}} : \mathbf{X} \in 2^{\mathbf{V}}\}) = \Lambda(\{\sigma_{\mathbf{X}} : \mathbf{X} \in 2^{\mathbf{V}} \setminus \mathbf{V}\}) + \sigma_{\mathbf{V}}. \quad (34)$$

In the odd cardinality case, $\Lambda(\{\sigma_{\mathbf{X}} : \mathbf{X} \in 2^{\mathbf{V}} \setminus \mathbf{V}\})$ is a sum of two positive operators and so we can conclude that it is positive, while in the even cardinality case, we cannot make this inference.

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- [51] In general, for those states whose triangle-incompatibility is distribution-witnessable by the Cut inflation, we do not expect *all* choices of local measurements to yield a distribution that witnesses this triangle-incompatibility. For instance, even though the triangle-incompatibility of the GHZ state is distribution-witnessable using the *AB*-Cut inflation by implementing a measurement of the computation basis on each qubit, it is not distribution-witnessable if one instead measures the $|+\rangle, |-\rangle$ basis on each qubit.
- [52] In its complex form, a semidefinite program can be formulated as

$$\begin{aligned} & \min_X \text{Tr}[Y_0 X] \text{ subject to} \\ & X \geq 0; \quad \text{Tr}[Y_i X] \leq b_i, i = 1, \dots, m, \end{aligned}$$

with X and the Y_i Hermitian for $i = 0, \dots, m$. In the case considered here, $I_{AB}(\rho_{ABC}(t))$ is Hermitian as it is a linear combination of Hermitian operators and the set S is convex (the partial transpose is a linear operation), which induces linear constraints on the variable Q_{ABC} .

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- [65] Regarding notation: the square-bracketed superscript is used here to have a way of labeling visible nodes with a numerical index rather than by using different letters. It is distinct to how round-bracketed superscripts have been used to label the factor spaces in a factorization of the Hilbert space of a latent node.
- [66] Recall that a set partition $\{\mathcal{S}_1, \dots, \mathcal{S}_k\}$ of a set $\mathcal{X}$ is a set of subsets of $\mathcal{X}$ such that $\cup_{i=1}^k \mathcal{S}_i = \mathcal{X}$ and $\mathcal{S}_i \cap \mathcal{S}_j = \emptyset$ for all $i \neq j \in \{1, \dots, k\}$.
- [67] The convention of considering index values greater than n or less than or equal to 0 to be taken modulo n is a convention that will be applied throughout this section and in the corresponding appendix, Appendix A 8. This also applies to set notation such as $\{j - l + 2, \dots, j\}$ if it corresponds to the possible values an index can take.
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