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Abstract

The constraints arising for a general set of causal relations, both classically and quantumly, are still poorly understood. As a step in exploring this question, we consider a *coherently controlled superposition* of ‘direct-cause’ and ‘common-cause’ relationships between two events. We propose an implementation involving the spatial superposition of a mass and general relativistic time dilation. Finally, we develop a computationally efficient method to distinguish such genuinely quantum causal structures from classical (incoherent) mixtures of causal structures and show how to design experimental verifications of the nonclassicality of a causal structure.

1. Introduction

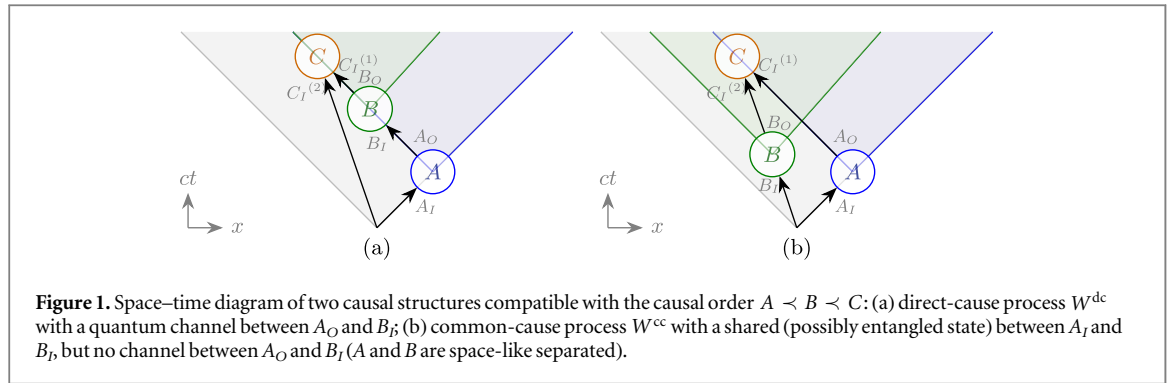
The deeply rooted intuition that the basic building blocks of the world are *cause-effect-relations* goes back over a thousand years [1–3] and yet still puzzles philosophers and scientists alike.

In physics, general relativity provides a theoretic account of the causal relations that describe which events in spacetime can influence which other events. For two (infinitesimally close) events separated by a time-like or light-like interval, one event is in the future light cone of the other, such that there could be a direct cause-effect relationship between them. When a space-like interval separates two events, no event can influence the other. The causal relations in general relativity are *dynamical*, since they are imposed by the dynamical light cone structure [4].

Incorporating the concept of causal structure in the quantum framework leads to novelties: it is expected that such a notion will be both *dynamical*, as in general relativity, as well as *indefinite*, due to quantum theory [5]. One might then expect indefiniteness with respect to the question of whether an interval between two events is time-like or space-like, or even whether event *A* is prior to or after event *B* for time-like separated events. Yet, finding a unified framework for the two theories is notoriously difficult and the candidate models still need to overcome technical and conceptual problems.

One possibility to separate conceptual from technical issues is to consider more general, *theory-independent* notions of causality. The *causal model* formalism [6, 7] is such an approach, which has found applications in areas as diverse as medicine, social sciences and machine learning [8]. The study of its quantum extension, allowing for non-local correlations [9–12] or including new information-theoretic principles [13–15] might provide intuitions and insights that are currently missing from the theory-laden take at combining quantum mechanics with general relativity.

Recently, it was found that it is possible to formulate quantum mechanics without any reference to a global causal structure [16]. The resulting framework—the *process matrix formalism*—allows for processes which are incompatible with any definite order between operations. One particular case of such a process is the ‘quantum switch’, where an auxiliary quantum system can coherently control the order in which operations are applied [17]. This results in a quantum controlled superposition of the processes ‘*A* causing *B*’ and ‘*B* causing *A*’. The quantum switch can also be realized through a preparation of a massive system in a superposition of two distinct states, each yielding a different but definite causal structure for future events [18, 19]. Furthermore, it provides



computational [20] and communication [21, 22] advantages over standard protocols with a fixed order of events. The first experimental proof-of-principle demonstration of the switch has been reported recently [23].

Given that one can implement superpositions of two different causal orders, one may ask if and how one could realize situations in which two events are in superpositions of being in ‘common-cause’ (A does not cause B directly) and ‘direct-cause’ (A and B share no common cause) relationships. Here we show that such superpositions exist and how to verify them.

We develop a framework for the computationally efficient verification of *coherent superpositions* of ‘direct-cause’ and ‘common-cause’ causal structures. We propose a natural physical realization of a quantum causal structure with the spatial superposition of a mass and general relativistic time dilation using the approach developed in [18, 19]. Finally, using the process matrix formalism, we define a degree of ‘nonclassicality of causal structures’ and show how to design *experimental verifications* thereof using a semidefinite program (SDP) [24].

2. Quantum causal models

To formalize the pre-theoretic notion of causality, the standard approach is to use *causal models* [6, 7], consisting of (i) a causal network and (ii) model parameters. The *causal network* is represented by a *directed graph*, whose nodes are variables and whose directed edges represent causal influences between variables. The causal influence from A to B is identified with the possibility of *signaling* from A to B . To exclude the possibility of causal loops, one imposes the condition that the graph should be *acyclic* (a ‘DAG’), which induces a *partial order* (‘causal order’) over the variables. The *model parameters* then determine how the probability distribution of each variable or set of variables is to be computed as a function of the value of its parent nodes.

Fully characterizing the causal model requires information which is available only through ‘interventions’, where the value of one or more variables is *set* to take a specific value, independently of the values of the rest of the variables. In the resulting causal network, the connections from all its parents are eliminated. Intervening on all relevant variables is sufficient to completely reconstruct the full causal model [7]. Since this is often practically impossible, it is crucial to investigate the possibilities of causal inference from a *limited* set of interventions.

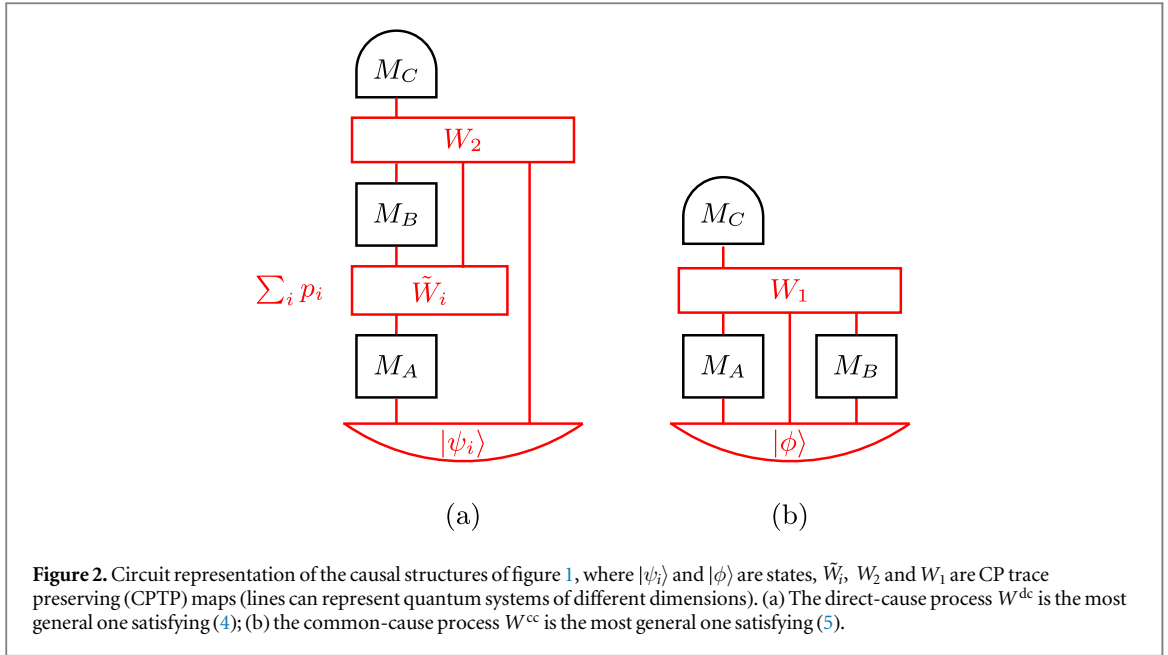
Moving to *quantum* causal models, we will define variables as results of generalized quantum operations applied to incoming quantum systems (‘local operation’). Formally, a local operation $\mathcal{M}_A : A_I \rightarrow A_O$ is a map from a density matrix $\rho_{A_I} \in A_I$ to $\rho_{A_O} \in A_O$ (where $A_I(A_O)$ denotes the space of linear operators on the Hilbert space \mathcal{H}^{A_I} (\mathcal{H}^{A_O})). The Choi–Jamiołkowski (CJ) isomorphism [25, 26] provides a convenient representation of the local map as a positive operator $M_A \in A_I \otimes A_O$ (the explicit definition is given in appendix A).

The *quantum causal structure*, which is the quantum analogue of the classical causal network, maps the aforementioned local operations to a probability distribution. It can be thought of as a *higher order operator* and can be formally represented in the ‘superoperator’, ‘quantum comb’ or ‘process matrix’ formalisms [16, 27–31].

We will focus on quantum causal structures with three laboratories (three nodes in the graph) A , B and C compatible with the causal order ‘ A is not after B , which is not after C ’ ($A \prec B \prec C$). This means that there are no causal influences from B and C to A , nor from C to B (see figure 1). (Since C is last, C ’s output space C_O can be disregarded.)

In the process matrix formalism, the quantum causal structure is represented by the matrix $W \in A_I \otimes A_O \otimes B_I \otimes B_O \otimes C_I$ [16, 32]. The probabilities of observing the outcomes i, j, k at A, B, C (corresponding to implementing the completely positive (CP) maps M_A^i, M_B^j, M_C^k respectively) are given by the *generalized Born rule*:

$$p(A = i, B = j, C = k) = \text{tr}[W(M_A^i \otimes M_B^j \otimes M_C^k)]. \quad (1)$$



The quantum causal structure and local operations should generate only meaningful (that is, *positive* and *normalized*) probability distributions. In addition, we require the probability distributions to be compatible with the causal order $A \prec B \prec C$. Note that both ‘common-cause’ and ‘direct-cause’ relationships between A and B are compatible with this causal order.

In terms of process matrices, these conditions are equivalent to requiring that W satisfies [32]:

$$W \geq 0, \quad W = \mathcal{L}_{A \prec B \prec C}(W), \quad (2)$$

$$\text{tr} W = d_{A_O} d_{B_O}. \quad (3)$$

$\mathcal{L}_{A \prec B \prec C}(\cdot)$ is the projection onto processes compatible with the causal order $A \prec B \prec C$, defined in appendix B. Equation (2) defines a convex cone \mathcal{W} , equation (3) a normalization constraint.

Following the standard DAG terminology, a purely ‘direct-cause’ process W^{dc} contains only a *direct cause-effect relation between A and B* , excluding any form of *common cause* between A and B . Any correlation between A and B is therefore caused by A alone (figures 1(a) and 2(a)). Tracing out C_I and B_O , the process matrix is a tensor product $\rho^{A_I} \otimes \tilde{W}^{A_O B_I}$. In our scenario, it will prove natural to *extend* this definition to include *convex mixtures* of direct-cause processes, i.e.,

$$\text{tr}_{C_I B_O} W^{\text{dc}} = \sum_i p_i \rho_i^{A_I} \otimes \tilde{W}_i^{A_O B_I}, \quad (4)$$

where $p_i \geq 0$, $\sum_i p_i = 1$, $\rho_i^{A_I}$ are arbitrary states and $\tilde{W}_i^{A_O B_I}$ arbitrary valid channels between Alice’s output and Bob’s input, representing to direct cause-effect links between A and B .

Such a process can be interpreted as a probability distribution over states entering A_I and corresponding channels from A_O to B_I . In the DAG framework, such probability distributions can be obtained from a graph with an additional latent node that acts as a common cause for all the observed nodes or simply ignorance of the graph that is implemented. Every channel from A to B with classical memory can be decomposed in this way; see appendix G for details.

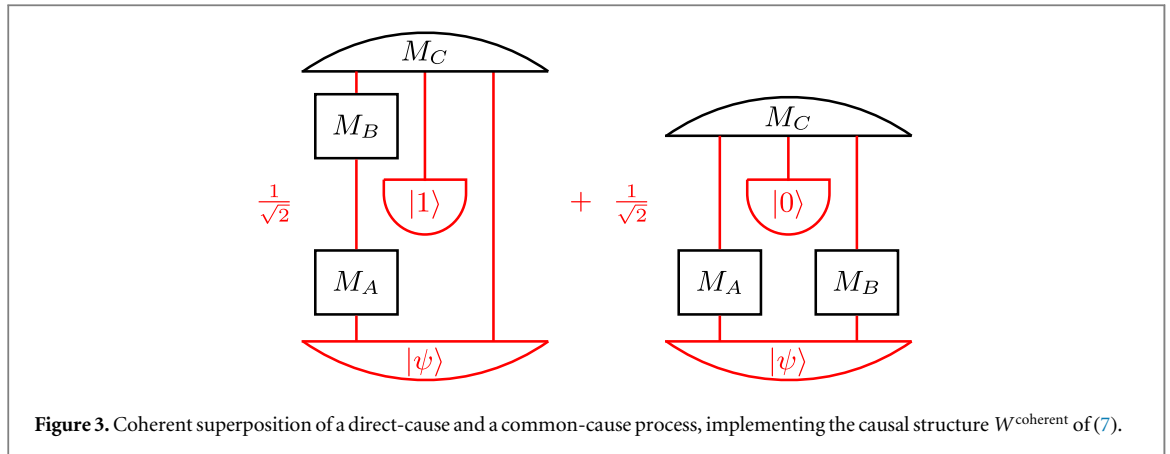
On the other hand, a purely ‘common-cause’ process W^{cc} does not include *any direct causal influence between A and B* (figures 1(b) and 2(b)). This implies that there is no channel between A_O and B_I . Therefore, when B_O and C_I are traced out, the process factorizes as

$$\text{tr}_{C_I B_O} W^{\text{cc}} = \sigma^{A_I B_I} \otimes \mathbb{1}^{A_O}, \quad (5)$$

where $\sigma^{A_I B_I}$ is an arbitrary (possibly entangled, possibly mixed) state, representing the common-cause influencing A and B .

3. Classical and quantum superpositions of causal structures

One possibility of combining direct-cause and common-cause processes consists in allowing for *classical mixtures* thereof: imagine that flipping a (possibly biased) coin determines which process will be realized in an experimental run. Formally, this is described by a process W^{conv} which can be decomposed as a convex



combination:

$$W^{\text{conv}} = qW^{\text{cc}} + (1 - q)W^{\text{dc}}, \quad (6)$$

where $0 \leq q \leq 1$, W^{dc} satisfies (4) and W^{cc} satisfies (5). Note that such a classical mixture was experimentally implemented in [33].

Can there be causal structures exhibiting *genuine quantum coherence*, i.e., that cannot be decomposed as a classical mixture of direct-cause and common-cause processes (while respecting the causal order $A \prec B \prec C$)? We now give an example of such a coherent superposition. It is analogous to the ‘quantum switch’ [17], which coherently superposes two causal orders $A \prec B \prec C$ and $B \prec A \prec C$, where the causal structure is entangled to a ‘control’ system $C_I^{(0)}$ added to C ’s input space³. To keep the notation simple, we define it in the ‘pure’ CJ-vector notation (see appendix A):

$$|w\rangle = \frac{1}{\sqrt{2}}(|0\rangle_{C_I^{(0)}} |\psi\rangle_{A_I B_I} |I\rangle_{A_O C_I^{(1)}} |I\rangle_{B_O C_I^{(2)}} + |1\rangle_{C_I^{(0)}} |\psi\rangle_{A_I C_I^{(2)}} |I\rangle_{A_O B_I} |I\rangle_{B_O C_I^{(1)}}),$$

$$W^{\text{coherent}} := |w\rangle \langle w|, \quad (7)$$

where $|I\rangle := \sum_{j=1}^d |jj\rangle$ represents a non-normalized maximally entangled state—the CJ-representation of an identity channel. The corresponding superposition of circuits is shown in figure 3. W^{coherent} satisfies neither the direct-cause condition (4) nor the common-cause condition (5) and is a projector on a pure vector, so it cannot be decomposed into *any nontrivial convex combination*, in particular not a mixture of direct-cause and common-cause processes. This proves that the process’s causal structure is nonclassical.

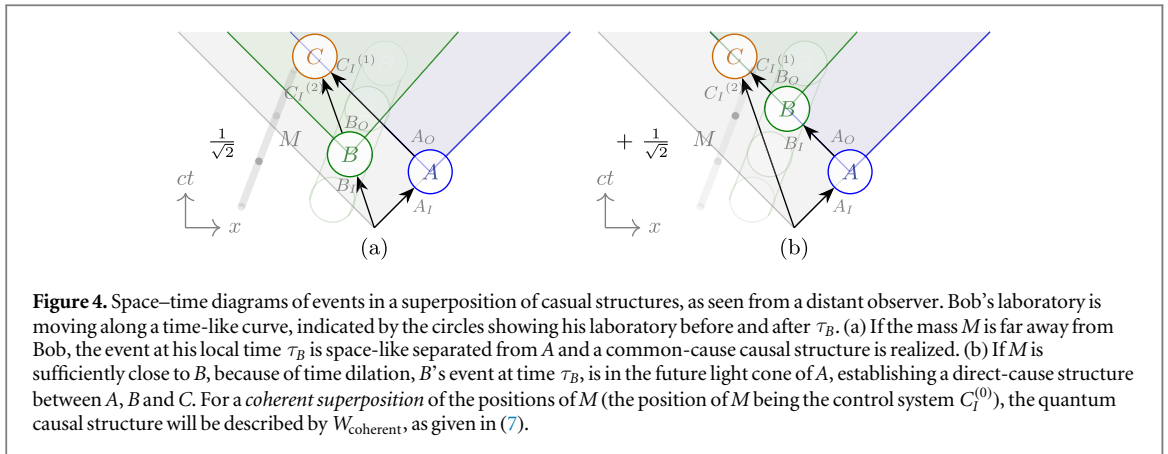
4. Physical implementation of the quantum causal structure

The causal structure W^{coherent} would not be of particular interest if it were a mere theoretical artifact. We now give an explicit and plausible physical scenario to realize the quantum causal structures in models which respect the principles of general relativistic time dilation and quantum superposition. We utilize the approach recently developed for the ‘gravitational quantum switch’ to realize a superposition and entanglement of two different causal orders [18, 19].

Consider two observers, Alice and Bob, who have initially synchronized clocks. We *define* the events in the respective laboratories with respect to the *local clocks*. Bob’s local operation will always be applied at his local time τ_B , while Alice’s is applied at her local time τ_A . We will consider two configurations, which will be controlled by a quantum system. The state of the control system is given by the position of a massive body. In the first configuration, all masses are sufficiently far away such that the parties are in an approximately flat spacetime. The events in the two laboratories are chosen such that the event B is outside of A ’s light cone and the common-cause causal relationship is implemented. The coordinate times of the two events, as measured by a local clock of a distant observer, are $t_A \approx \tau_A$ and $t_B \approx \tau_B$. (figure 4(a)).

In the second configuration, a mass M is put closer to Bob’s laboratory than to Alice’s such that his clock runs slower with respect to hers due to gravitational time dilation. With a suitable choice of mass and distance between Alice and Bob, the event B , which is defined by his clock showing local time τ_B , will be inside A ’s future light cone. In terms of coordinate times one now has $t'_A = \tau_A / \sqrt{-g_{00}(A)}$ and $t'_B = \tau_B / \sqrt{-g_{00}(B)}$, where

³ See [34] for a different type of quantum causal structure proposed independently.



$g_{00}(A)$ and $g_{00}(B)$ are the ‘00’ components of the metric tensor at the position of the laboratories. This configuration can implement the direct-cause relationship (figure 4(b)).

If the mass M is initially in a coherent *spatial superposition* of a position close and a position far away from Bob, the quantum superposition of causal structures W_{coherent} is implemented. The *position of the mass* acts as the control system $C_I^{(0)}$; it can be received by Charlie, who can manipulate it further (in particular, measure it in the superposition basis). Any possible information about the causal structure (direct cause or common cause) encoded in the degrees of freedom of the laboratories, such as for example in the clocks of the labs, must be erased, possibly using the methods of [19].

Note that, in contrast to the superposition of different causal orders [18, 19], the time dilation necessary to ‘move B in or out’ of the light cone can, in principle, be made *arbitrarily small*, if Bob can define τ_B and thus the event B with a sufficiently precise clock⁵.

To give an idea of the orders of magnitude involved: for a spatial superposition of the order of $\Delta x = 1$ mm and a mass of $M = 1$ g, Bob’s clock should resolve one part in 10^{27} to be able to certify the nonclassicality of the causal structure. This regime is still quite far from experimental implementation, since the best molecule interferometers [35] do not go beyond $M = 10^5$ amu, $\Delta x = 10^{-6}$ m, while the best atomic lattice clocks achieve a precision of one part in 10^{18} [36]. An additional difficulty consists in avoiding significant entanglement between the position of the mass and systems other than the local clocks. Nonetheless, this regime is still far away from the Planck scale that is usually assumed to be relevant for quantum gravity effects.

We also stress that the process W_{coherent} , although it cannot be decomposed as a convex combination of a common cause and a direct cause process, is still compatible with the causal order $A \prec B \prec C$ and, as such [37], can be realized as a quantum circuit, as shown in figure B1(b) of appendix B.

5. Verifying the nonclassicality of causal structures

We now provide an *experimentally accessible* and *efficiently computable* measure of the nonclassicality of causality.

Let us first define the set \mathcal{S} of operators which are positive on any convex combination W^{conv} of direct-cause and common-cause processes (i.e., processes satisfying (6)):

$$S \in \mathcal{S} \Rightarrow \text{tr}[S W^{\text{conv}}] \geq 0 \quad \forall W^{\text{conv}}. \quad (8)$$

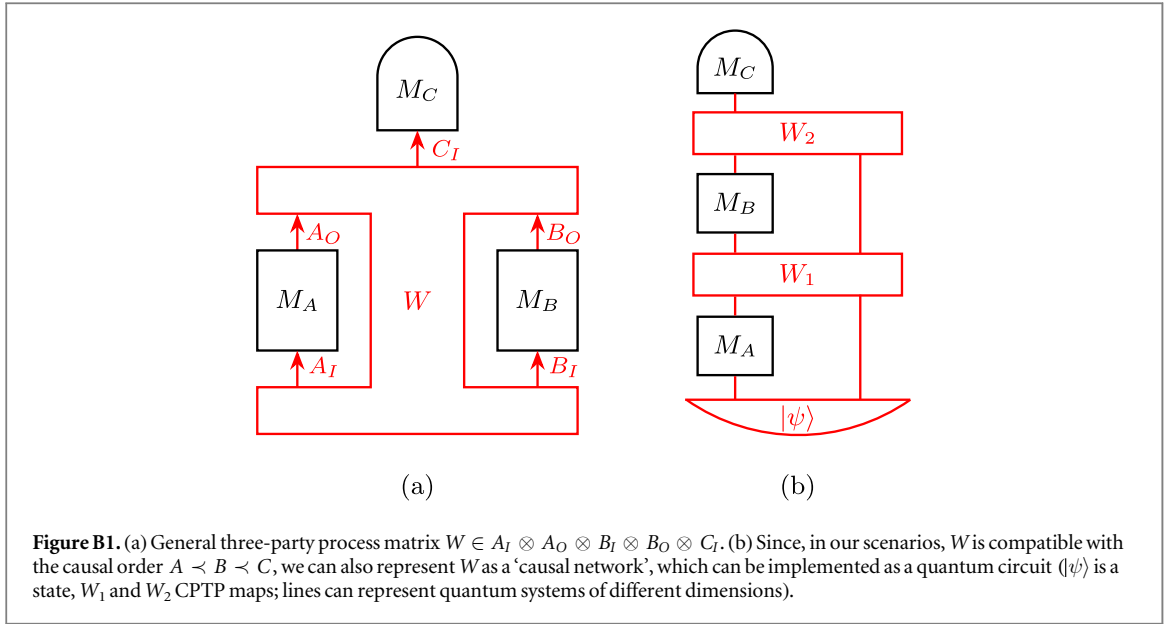
If S is positive on all convex combinations of direct-cause and common-cause process matrices, then it is also positive on all direct-cause ($\text{tr}[S W^{\text{dc}}] \geq 0$) and common-cause ($\text{tr}[S W^{\text{cc}}] \geq 0$) processes individually.

Since W^{dc} is a direct-cause process (4) if and only if the operator $\text{tr}_{C_I B_O} W^{\text{dc}}$ is separable with respect to the bipartition $(A_I, A_O B_I)$, we effectively require S to be an *entanglement witness* [38, 39] of the reduced process for the bipartition $(A_I, A_O B_I)$. The full characterization of the set of entanglement witnesses is known to be computationally hard [40]. Instead, we will use the *positive partial transpose* [41, 42] criterion as a relaxation to define an efficiently computable measure of nonclassicality.

Enforcing the condition that S is positive on common-cause process matrices in terms of semidefinite constraints is straightforward: since the condition for W^{cc} (5) to be a common-cause process is already a

⁴ The state $|0\rangle$ corresponding to the mass being far away from Bob and the state $|1\rangle$ corresponding to the mass being close to Bob.

⁵ If Bob’s clock cannot resolve the interval $\tau_B(1 - 1/\sqrt{-g_{00}(B)})$ within the time τ_B , the event B will be inside or outside A ’s light cone randomly and independently of the position of M , adding noise to the process.



semidefinite constraint, the ‘dual’ constraint for S to be positive on all common-cause process matrices is semidefinite as well.

The operators in the set \mathcal{S}_{SDP} (explicitly constructed in appendix D) are defined as those that obey *both* the condition of having a positive partial transpose and being positive on all common-cause process matrices. Every $S \in \mathcal{S}_{\text{SDP}}$ has positive trace with any W^{conv} . Conversely, $\text{tr}[S W] < 0$ certifies that the process W is a genuinely nonclassical causal structure—the operators S can therefore be used as *nonclassicality of causality witnesses*⁶.

It is crucial to realize that for every given genuinely quantum W , one can *efficiently optimize*—the optimization is a SDP [24]—over the set of nonclassicality witnesses to find the one that has minimal trace with W :

$$\begin{aligned} & \min \text{tr}[S W] \\ \text{s.t. } & S \in \mathcal{S}_{\text{SDP}}, \quad \mathbb{1}/d_O - S \in \mathcal{W}^*, \end{aligned} \quad (9)$$

where \mathcal{W}^* is the dual cone of \mathcal{W} , given in appendix C. The *normalization condition* $\mathbb{1}/d_O - S \in \mathcal{W}^*$ is necessary for the optimization to reach a finite minimum and confers an operational meaning to $\mathcal{C}(W) := -\text{tr}[S_{\text{opt}} W]$: it is the amount of ‘worst-case noise’ the process can tolerate before its quantum features stop being detectable by witnesses in \mathcal{S}_{SDP} (in analogy to the ‘generalized robustness of entanglement’ [43]). Because of its ability to certify the quantum nonclassicality of causal structures, we will refer to $\mathcal{C}(\cdot)$ as the ‘nonclassicality of causality’. Note that $\mathcal{C}(\cdot)$ satisfies the natural properties of *convexity* and *monotonicity under local operations* (see appendix E).

To experimentally verify the properties of a process like W^{coherent} , one can use the SDP (9) to compute the optimal nonclassicality of causality witness S_{opt} for W^{coherent} . The nonclassicality of causality $\mathcal{C}(W^{\text{coherent}})$ can be measured by decomposing S_{opt} in a convenient basis of local operations. In general, this is as demanding as performing a full ‘causal tomography’ [15, 32, 33].

6. Causal inference under experimental constraints

There are two reasons to consider witnesses that are subject to certain *additional restrictions*. First, there might be various technical limitations arising from the experimental setup [23, 33], which make full tomography impractical. Second, in analogy to the classical case, it is of *conceptual* interest to investigate the power of *quantum causal inference mechanisms* working on *limited data*. In particular, one might want to investigate differences between quantum and classical causal inference algorithms under such constraints.

As an application of this method, we will examine witnesses for the process W^{coherent} . In the following, we will consider qubit input and output spaces, i.e., $\dim A_I = \dim A_O = \dim B_I = \dim C_I^{(0,1,2)} = 2$ for simplicity and computational speed. The optimal witness for W^{coherent} , obtained from the optimization (9) using YALMIP [44] with the solver MOSEK⁷, leads to a nonclassicality of causality of $\mathcal{C}(W^{\text{coherent}}) = -\text{tr}[S_{\text{opt}} W^{\text{coherent}}] \approx 0.2278$.

⁶ The ‘causal witnesses’ introduced in [32] are conceptually different, since they examine whether a process can be decomposed as a convex mixture of *causally ordered* processes. All of the processes we study here have a fixed causal order $A \prec B \prec C$.

⁷ The MOSEK optimization toolbox for MATLAB, version 7.0.

An intriguing feature of quantum causal models is that direct-cause correlations (figure 1(a)) and common-cause correlations (figure 1(b)) can be distinguished through a restricted class of informationally symmetric operations [31], sometimes called ‘observations’ [33, 45] that are non-demolition measurements (we refer the reader to appendix H for certain issues with this definition). We can constrain a witness S^{ndmeas} to consist of linear combinations of such non-demolition measurements through an additional condition to the SDP (9), given in appendix F.

Surprisingly, purely ‘observational’ witnesses are sufficient not only to distinguish common-cause from direct-cause processes, but *also* to distinguish a classical mixture of direct-cause and common-cause processes from a genuine quantum superposition, since $-\text{tr}[S_{\text{opt}}^{\text{ndmeas}} W_{\text{coherent}}] \approx 0.0732$.

Since measurements and preparations and even non-demolition measurements are often challenging to implement [46], it can also be useful to consider a nonclassicality of causality witness S^{unitary} which can be decomposed into *unitary operations* for A and B , and arbitrary measurements for C . The requirement can also easily be translated in a semidefinite constraint, given in appendix F. One finds that $-\text{tr}[S_{\text{opt}}^{\text{unitary}} W_{\text{coherent}}] \approx 0.1686$. A summary of the different constraints mentioned in this section can be found in appendix F.

7. Conclusions

We presented a three-event quantum causal model compatible with the causal order $A \prec B \prec C$ which is a quantum controlled *coherent superposition between common-cause and direct-cause models*, not a classical mixture thereof.

The experimental implementation we proposed is of conceptual interest, since it relies both on general relativity and the quantum superpositions principle, two elements we expect to feature in a full theory unifying quantum theory and general relativity. Interestingly, both the mass of the object and the separation between the two amplitudes can be arbitrarily small, as long as Bob has access to a sufficiently precise clock to define the instant of his event B .

In order to experimentally certify a genuinely quantum causal structure, we introduced and characterized *nonclassicality of causality witnesses* and provided a SDP to efficiently compute them. Experimental and conceptual constraints are readily included in the framework.

The potential of quantum causal structures as a quantum information resource was recently demonstrated in terms of query complexity [20] and communication complexity [21, 22], but is still poorly understood. It would be interesting to understand which advantages could be obtained from the coherent superpositions of and common- and direct-cause processes.

Remark. In the final stages of completing this manuscript, a related work by MacLean *et al* [34] appeared independently. The difference in the definitions of direct-cause processes between the two papers and its implications are discussed in appendix G.

Acknowledgments

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Appendix A. CJ isomorphism

The CJ representation of a CP map $\mathcal{M}_A: A_I \rightarrow A_O$ is

$$M_A := [(\mathcal{I} \otimes \mathcal{M}_A)(|I\rangle\rangle\langle\langle I|)]^T \in A_I \otimes A_O, \quad (\text{A1})$$

where \mathcal{I} is the identity map, $|I\rangle\rangle := \sum_{j=1}^{d_{\mathcal{H}_I}} |jj\rangle \in \mathcal{H}_I \otimes \mathcal{H}_I$ is a non-normalized maximally entangled state and T denotes matrix transposition in the computational basis.

The inverse transformation is then defined as:

$$\mathcal{M}_A(\rho) = \text{tr}_I[(\rho \otimes \mathbb{1})M_A]^\Gamma. \quad (\text{A2})$$

For operations which have a single Kraus operator ($\mathcal{M}_A(\rho) = A\rho A^\dagger$), one also define a ‘pure CJ-isomorphism’ [47, 48], which maps the operation to a *vector*⁸:

$$|A^*\rangle := (\mathbb{1} \otimes A^*)|I\rangle \in \mathcal{H}^{A_I} \otimes \mathcal{H}^{A_O}. \quad (\text{A3})$$

The usual CJ-representation of such an operation is simply the *projector onto the CJ-vector*: $M_A = |A^*\rangle\langle A^*|$.

Appendix B. Causally ordered and common-cause process matrices

We first introduce a shorthand that we will use throughout the following appendices:

$${}_X W := \frac{\mathbb{1}^X}{d_X} \otimes \text{tr}_X W, \quad (\text{B1})$$

where d_X is the dimension of the Hilbert space X .

In this paper, we consider three parties, where the C ’s output space C_O can be disregarded. The process matrix $W \in A_I \otimes A_O \otimes B_I \otimes B_O \otimes C_I$, which encodes the quantum causal model, is defined on the dual space to the tensor products of the maps. Since both the ‘common-cause’ and the ‘direct-cause’ scenarios are compatible with the causal order $A \prec B \prec C$, we can also represent the process matrix W as a circuit. (See figure B1.)

For instance, the coherent superposition of common cause and direct cause, defined in (7), would consist of $|\psi\rangle = |\phi^+\rangle \otimes (|0\rangle + |1\rangle)/\sqrt{2}$, W_1 and W_2 being control-SWAPs (where the control is the last qubit, initially in the state $(|0\rangle + |1\rangle)/\sqrt{2}$).

We now define the projection $\mathcal{L}_{A \prec B \prec C}(\cdot)$ onto the linear subspace of process matrices compatible with the causal order $A \prec B \prec C$, which can be derived from the conditions given in [32]:

$$\mathcal{L}_{A \prec B \prec C}(W) := W -_{C_I} W +_{B_O C_I} W -_{B_I B_O C_I} W +_{A_O B_I B_O C_I} W. \quad (\text{B2})$$

$W^{A \prec B \prec C}$ is compatible with the causal order $A \prec B \prec C$ if and only if $W^{A \prec B \prec C} = \mathcal{L}_{A \prec B \prec C}(W^{A \prec B \prec C})$ holds.

The projection onto the subspace of common-cause process matrices $\mathcal{L}_{cc}(\cdot)$ is given by composing the projection $\mathcal{L}_{A \prec B \prec C}$ with the projection onto processes which have no channel from A_O to B_I :

$$\mathcal{L}_{cc}(W) := \mathcal{L}_{A \prec B \prec C}(W) -_{C_I} \mathcal{L}_{A \prec B \prec C}(W) +_{C_I A_O} \mathcal{L}_{A \prec B \prec C}(W). \quad (\text{B3})$$

Appendix C. Dual cones

Given the definition (2) of the cone \mathcal{W} , we can characterize the *dual cone* \mathcal{W}^* of all operators whose product with operators in \mathcal{W} has positive trace. Remember that \mathcal{W} is the *intersection* of the cone of positive operators \mathcal{P} with a linear subspace defined by the conditions for causal order: $\mathcal{W} := \mathcal{P} \cap \mathcal{L}_{A \prec B \prec C}$.

The dual of the linear subspace $\mathcal{L}_{A \prec B \prec C}^*$ is its orthogonal complement [24, 32]

$$\mathcal{L}_{A \prec B \prec C}^* = \mathcal{L}_{A \prec B \prec C}^\perp, \quad (\text{C1})$$

i.e., the space of operators with a support that is orthogonal to the original subspace.

Additionally, the dual of the intersection of two closed convex cones containing the origin is the convex union of their duals [24, 32], so that

$$\mathcal{W}^* = (\mathcal{P} \cap \mathcal{L}_{A \prec B \prec C})^* = \text{conv}(\mathcal{P}^* \cup \mathcal{L}_{A \prec B \prec C}^\perp). \quad (\text{C2})$$

Since the cone of positive operators is self-adjoint ($\mathcal{P}^* = \mathcal{P}$), we can combine (C1) and (C2) into $\mathcal{W}^* = \text{conv}(\mathcal{P} \cup \mathcal{L}_{A \prec B \prec C}^\perp)$. Explicitly, this means that any operator $Q \in \mathcal{W}^*$ can be decomposed as

$$\begin{aligned} Q &= Q_1 + Q_2 \\ \text{s.t. } Q_1 &\geq 0, \quad \mathcal{L}_{A \prec B \prec C}(Q_2) = 0. \end{aligned} \quad (\text{C3})$$

Appendix D. Nonclassicality of causality witnesses

We will now explicitly construct the set of nonclassicality of causality witnesses \mathcal{S}_{SDP} .

⁸ Note that there are differing conventions, where the conjugation is omitted.

The semidefinite relaxation of the direct-cause constraint (4) in terms of positive partial transposition is (using the shorthand introduced in (B1)):

$$({}_{C_I B_O} W^{\text{dc}})^{T_{A_I}} \geq 0. \quad (\text{D1})$$

The dual cone (D2) to the cone of relaxed direct-cause processes defined by the intersection of \mathcal{W} with the cone defined in (D1). The dual cone (D3) to the cone of common-cause processes defined by the intersection of \mathcal{W} with the linear subspace (5) can be constructed in the same way as in appendix C.

The set of witnesses positive on all positive partial transpose operators is a *subset* of entanglement witnesses. Any witness belonging to this set satisfies⁹:

$$\begin{aligned} S^{\text{dc}} &= {}_{C_I B_O}(S_1^{T_{A_I}}) + S_2 + S_3 \\ \text{s.t. } S_1, S_2 &\geq 0, \quad \mathcal{L}_{A \prec B \prec C}(S_3) = 0. \end{aligned} \quad (\text{D2})$$

If $\text{tr}[S^{\text{dc}} W] < 0$, this implies that W is not a direct-cause process as defined in equation (4). Note that since we are only considering a subset of entanglement witnesses, *the converse does not hold*.

We can now turn to the requirement that S is positive on common-cause processes. Since condition (5) (corresponding to (B3) together with positivity) defines a convex cone, we can use the techniques of appendix C to construct the dual cone, of which the witness will be an element. This leads us to write S^{cc} as

$$\begin{aligned} S^{\text{cc}} &= S_4 + S_5 \\ \text{s.t. } S_4 &\geq 0, \quad \mathcal{L}_{\text{cc}}(S_5) = 0, \end{aligned} \quad (\text{D3})$$

where the projection onto the common-cause subspace \mathcal{L}_{cc} is defined in appendix B. W is *not* a common-cause process as defined in (4) if and only if there exists an S^{cc} such that $\text{tr}[S^{\text{cc}} W] < 0$.

Now, combining both conditions, we can construct a set of operators positive on all mixtures of direct-cause and common-cause processes *only in terms of semidefinite constraints*. To test whether an arbitrary W process is of this type, we can run the following SDP [24]:

$$\begin{aligned} &\min \text{tr}[S W] \\ \text{s.t. } S &= {}_{C_I B_O}(S_1^{T_{A_I}}) + S_2 + S_3 = S_4 + S_5, \\ S_1 &\geq 0, \quad S_2 \geq 0, \quad S_4 \geq 0, \\ \mathcal{L}_{A \prec B \prec C}(S_3) &= \mathcal{L}_{\text{cc}}(S_5) = 0, \\ \mathbb{1}/d_O - S &\in \mathcal{W}^*. \end{aligned} \quad (\text{D4})$$

The last condition, where \mathcal{W}^* is the cone dual to \mathcal{W} (see appendix C), imposes a normalization on S . It gives the nonclassicality of causality $\mathcal{C}(W) = -\text{tr}[S_{\text{opt}} W]$ the operational meaning of ‘generalized robustness’, quantifying resistance of the nonclassicality detectable by \mathcal{S}_{SDP} to *worst possible noise* [32, 43]. This becomes more intuitive from the dual SDP, given by

$$\begin{aligned} &\min \text{tr}[\Omega/d_O] \\ \text{s.t. } W + \Omega &= W^{\text{cc}} + W^{\text{dc}}, \\ ({}_{C_I B_O} W^{\text{dc}})^{T_{A_I}} &\geq 0, \quad W^{\text{dc}} \in \mathcal{W}, \\ {}_{C_I} W^{\text{cc}} = {}_{C_I A_O} W^{\text{cc}}, &\quad W^{\text{cc}} \in \mathcal{W}. \end{aligned} \quad (\text{D5})$$

The process $\Omega \cdot d_O / \text{tr}[\Omega]$ can be interpreted as worst-case noise with respect to the optimal witness S_{opt} , resulting from the SDP (D4).

Appendix E. Convexity and monotonicity

Here we prove that the *nonclassicality of causality* defined as $\mathcal{C}(W) := -\text{tr}[S_{\text{opt}} W]$, which results from the SDP (D4), satisfies the natural properties of *convexity* and *monotonicity*, following analogous proofs of [32].

Convexity means that $\mathcal{C}(\sum_i p_i W_i) \leq \sum_i p_i \mathcal{C}(W_i)$, for any $p_i \geq 0$, $\sum_i p_i = 1$. Take S_{W_i} to be the optimal witness for W_i . Any other witness, in particular the optimal witness S_W for $W := \sum_i p_i W_i$ will be less robust to noise with respect to W_i :

$$\text{tr}[S_{W_i} W_i] \leq \text{tr}[S_W W_i]. \quad (\text{E1})$$

⁹We included the term S_2 and S_3 although they do not make the witnesses ‘more powerful’ to detect entanglement. S_2 will become relevant when combining the conditions on direct-cause and common-cause processes in equation (D4); S_3 is included because it could appear in restricted types of witnesses [32].

Averaging over i we have

$$-\text{tr} \left[S_W \sum_i p_i W_i \right] \leq -\sum_i p_i \text{tr}[S_{W_i} W_i], \quad (\text{E2})$$

which is exactly the statement of convexity for \mathcal{C} .

Monotonicity under local operation means that $\mathcal{C}(W) \geq \mathcal{C}(\$ (W))$, where $\$(\cdot)$ is the composition of W with local operations.

We wish to show that $-\text{tr}[S_{\$(W)} \$ (W)] \leq -\text{tr}[S_W W]$. By duality, this is equivalent to

$$-\text{tr}[\$^*(S_{\$(W)}) W] \leq -\text{tr}[S_W W], \quad (\text{E3})$$

where $\$^*(\cdot)$ is the map dual to $\$(\cdot)$. Equation (E3) is satisfied if $\$^*(S_{\$(W)})$ is a witness, i.e., is positive on all mixtures of direct-cause and common-cause operators ($\text{tr}[\$^*(S_{\$(W)}) W^{\text{mix}}] \geq 0$), and is normalized appropriately ($\mathbb{1}/d_O - \$^*(S_{\$(W)}) \in \mathcal{W}^*$).

The first condition can be seen to hold by applying duality and using the fact that local operations map any mixture of direct-cause and common-cause processes to a mixture of direct-cause and common-cause processes. The second condition is equivalent to

$$\text{tr}[\mathbb{1}/d_O - \$^*(S_{\$(W)}) \Omega] \geq 0 \quad (\text{E4})$$

for every process matrix Ω . We apply duality and linearity of the trace to find that

$$\text{tr}[S_{\$(W)} \$ (\Omega)] \leq \text{tr}[\Omega]/d_O. \quad (\text{E5})$$

This relation holds because $\$(\cdot)$ maps normalized ordered process matrices to normalized ordered process matrices and $\mathbb{1}/d_O - S_{\$(W)} \in \mathcal{W}^*$ is the normalization condition for the SDP (D4).

The condition of *discrimination* (or *faithfulness*), which would mean that $\mathcal{C}(W) \geq 0$ if and only if the process matrix is not a mixture of direct-cause and common-cause processes (6), is *not satisfied*. Since we relied on a relaxation of the direct-cause condition by using the positive partial transpose criterion, there are processes which are not a mixture satisfying (6) but for which the nonclassicality of causality is zero.

Therefore, the nonclassicality of causality is not a *faithful measure* of the nonclassicality of the causal structure. This is reasonable, since finding such a measure would be equivalent to finding a fully general *entanglement criterion*—a problem known to be computationally hard [40].

Appendix F. Experimental constraints on witnesses

In this appendix, we give the explicit form of the experimental constraints mentioned in the main text. When using a constrained class of witnesses, the value $-\text{tr}[S_{\text{opt}}^{\text{restricted}} W_{\text{coherent}}]$ can be interpreted as the *amount of noise* tolerated before the *constrained set of witnesses* becomes incapable of detecting the nonclassicality of causality of W_{coherent} .

A simple example of a restriction simplifying the experimental implementation consists in disregarding the space $C_I^{(1,2)}$, i.e., to have $S=C_I^{(1,2)}$ as an additional constraint. The nonclassicality of causality is *unaffected* by this restriction, which shows that the input spaces $C_I^{(1,2)}$ do not carry any additional information about the nonclassicality of causality.

The constraint for the witness to consist only of non-demolition measurements is

$$S^{\text{ndmeas}} = \sum_{ijl} \alpha_{ijl} (\mathbb{1} + \sigma_i^{A_l}) \otimes (\mathbb{1} + \sigma_i^{A_o}) \otimes (\mathbb{1} + \sigma_j^{B_l}) \otimes (\mathbb{1} + \sigma_j^{B_o}) \otimes E_l^{C_i}, \quad (\text{F1})$$

where σ_k ($k = 1, 2, 3$) are the qubit Pauli matrices and E_l , $l = 1, \dots, 8$ is an arbitrary basis of projectors on C_I 's three qubits.

The constraint for the witness to only consist of unitary operations¹⁰ for A and B is:

$$S^{\text{unitary}} = \sum_{ijl} \beta_{ijl} |U_i^*\rangle \langle U_i^{*A_l A_o} \otimes |U_j^*\rangle \langle U_j^{*B_l B_o} \otimes E_l^{C_i}, \quad (\text{F2})$$

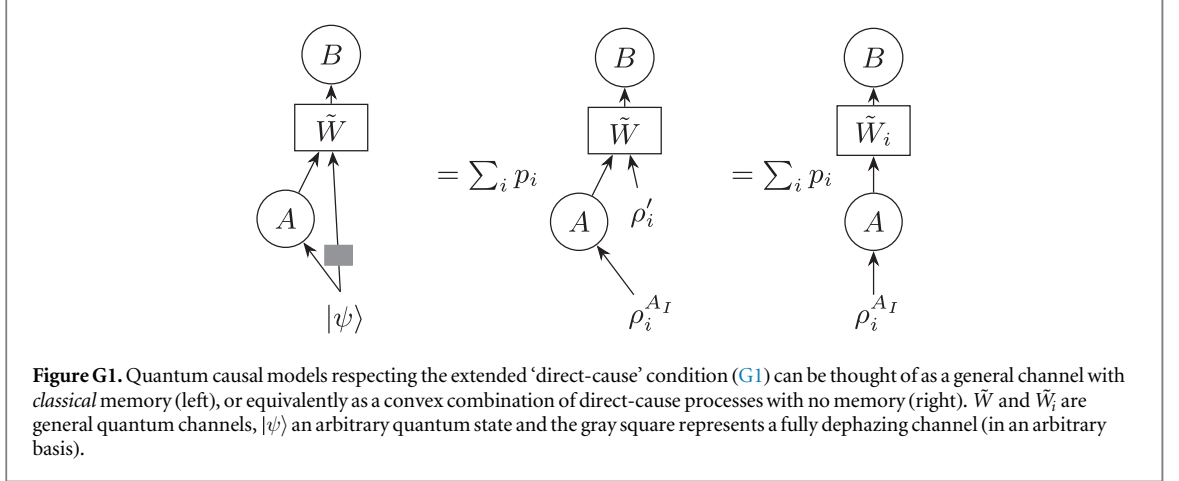
where $i, j = 1, \dots, 10$ indexes a basis¹¹ of the CJ-vectors (see appendix A) of unitaries. See table F1 for the amount of noise tolerated by different constrained sets of witnesses.

¹⁰ Note that according to definition of [33], unitary witnesses should also be considered as ‘observations’ although operationally they are standardly understood as interventions.

¹¹ This is because there are ten linearly independent projectors on CJ-vectors for unitaries acting on qubits [32].

Table F1. Constrained nonclassicality of causality for different types of constraints on S , in descending order.

Constraint on the witness S	$-\text{tr}[S W^{\text{coherent}}]$
No constraint	0.2278
Discarding $C_I^{(1,2)}$	0.2278
Unitary operations A, B	0.1686
ND measurement A, B	0.0732



Appendix G. Definition of direct-cause processes and relationship to the definitions of [34]

Since [34] considers the two party case, we can merge B and C to make our scenario comparable to the one of [34]. More precisely, B_I and C_I are relabeled as B'_I and B_O is disregarded, eliminating the necessity to trace over B_O and C_I . The condition for direct-cause processes (4) then becomes

$$W^{\text{dc}} = \sum_i p_i \rho_i^{A_I} \otimes \tilde{W}_i^{A_O B'_I}, \quad (\text{G1})$$

which implies that the states given to A and the channel connecting A and B can be *classically correlated*.

In the terminology of DAGs this convex mixture would correspond to tracing over a (hidden) classical¹² common cause between A and B . An alternative, more restricted definition would exclude such classical correlations, i.e.,

$$W^{\text{dc}} = \rho^{A_I} \otimes \tilde{W}^{A_O B'_I}, \quad (\text{G2})$$

is used in [34]. To make the difference apparent, consider the convex mixture of two direct-cause processes between A and B (here, $\dim A_I = \dim A_O = \dim B'_I = 2$):

$$W^{\text{mem}} = \frac{1}{4} |0\rangle \langle 0|^{A_I} (\mathbb{1}^{A_O B'_I} + \sigma_z^{A_O} \sigma_z^{B'_I}) + \frac{1}{4} |1\rangle \langle 1|^{A_I} (\mathbb{1}^{A_O B'_I} - \sigma_z^{A_O} \sigma_z^{B'_I}), \quad (\text{G3})$$

where the tensor products between the Hilbert spaces are implicit. W^{mem} classically correlates the channel between A_O and B'_I (a classical channel with or a without bit flip) to the state in A_I , as shown in figure G1. It is of the type (G1) but *not* of the type (G2).

In [34], (G3) is not considered to be a direct-cause process, nor a convex mixture (called ‘probabilistic mixture’) of direct-cause and common-cause processes. It is instead termed a ‘physical mixture’ of common-cause and direct-cause processes.

We instead use the broader definition (G1) because we ultimately intend to study convex combinations of common-cause and direct-cause processes (6), which means we should also allow for convex combinations of direct-cause processes. The restricted definition (G2) for direct-cause processes would lead to consider a convex combination of a direct-cause and a common-cause process to be a ‘probabilistic mixture’, but *not* a convex combination of *two cause-effect processes*.

¹²Strictly speaking, it just needs not to produce any entanglement between A_I and (A_O, B_I) , see figure G1.

Finally note that the class of processes, which, when post-selected on CP maps being implemented at B'_I , result in an entangled conditional process on $A_I A_O$, is defined to be ‘coherent mixtures’ in [34]. All of these ‘coherent mixtures’ are nonclassical in our terminology (the processes that can be decomposed as (6) never result in an entangled conditional process on $A_I A_O$). It is not clear whether the converse is true.

Appendix H. Issues in defining a quantum ‘observational scheme’

Ried *et al* [33] define the ‘observational scheme’ (as opposed to the ‘interventionist scheme’) on a quantum causal structure as composed of operations satisfying the ‘informational symmetry principle’. We examine the subtleties and issues involved in this definition, in particular regarding the dependence on the initially assigned state.

Reference [33] assumes that before the observation, one assigns the (epistemic) state ρ_{A_I} to the system coming into A ’s laboratory. A quantum operation (described by the CJ representation of the quantum instrument [49] $\{M_A^i\}$, where i labels the outcome) is applied. This updates the information about the outgoing state $\rho_{A_O}^{(i)}$ but also (through retrodiction) about the incoming state $\rho_{A_I}^{(i)}$. These states are found by applying the update rules [31]

$$\rho_{A_O}^{(i)} = \frac{\text{tr}_{A_I}[M_A^i \cdot \rho_{A_I} \otimes \mathbb{1}_{A_O}]^{\Gamma}}{\text{tr}[M_A^i \cdot \rho_{A_I} \otimes \mathbb{1}_{A_O}]}, \quad (\text{H1})$$

$$\rho_{A_I}^{(i)} = \frac{\text{tr}_{A_O}[(\sqrt{\rho_{A_I}} \otimes \mathbb{1}_{A_O})M_A^i(\sqrt{\rho_{A_I}} \otimes \mathbb{1}_{A_O})]}{\text{tr}[(\sqrt{\rho_{A_I}} \otimes \mathbb{1}_{A_O})M_A^i(\sqrt{\rho_{A_I}} \otimes \mathbb{1}_{A_O})]}. \quad (\text{H2})$$

The informational symmetry principle holds if and only if after the operation, the states assigned to the incoming and outgoing systems are the same:

$$\rho_{A_I}^{(i)} = \rho_{A_O}^{(i)}. \quad (\text{H3})$$

For Ried *et al*, an instrument for which this informational symmetry holds is *defined* to be an ‘observation’ [33]. In this sense, there can obviously be ‘non-passive’ observations such as non-demolition measurements. Any non-demolition measurement in a basis in which the initially assigned state ρ_{A_I} is *diagonal* will be an observation in this sense. This matches the intuition that a *classical* measurement only *reveals* information and does not disturb the system.

If one wishes to implement measurements in *arbitrary bases*, the *only* initially assigned state which results in informational symmetry is the maximally mixed state $\rho_{A_I} = \mathbb{1}/d$ [33]. This shows how problematic the definition of observational scheme is, since it not only crucially depends on an initial (epistemic) assignment ρ_{A_I} but also because there is *only one* such assignment which allows all measurements to be ‘observations’—which tolerates no amount and no type of noise. In this sense, as soon as the experimenter *changes her beliefs* about the incoming state *in any way*, she will be intervening on the system, not merely observing it.

Leaving aside these interpretative difficulties, it is interesting to realize that operations which are *unitary* also turn out to be ‘observations’ if the initially assigned state is $\rho_{A_I} = \mathbb{1}/d$: for a unitary operation, $\rho_{A_I}^{(i)} = \rho_{A_O}^{(i)} = \rho_{A_I} = \mathbb{1}/d$. The unitary provides exactly the same information about input and output states, namely *none*.

Finally, note that both the framework of [33] and the one we developed rely on the assumption that quantum theory is valid and the correct operations were implemented—the analysis is *device-dependent*. This means that any ‘quantum advantage’ in inference will not be based on *mere correlations* in the sense of a conditional probability distribution of outputs given inputs. This makes the comparison with the power of classical causal models somewhat problematic.

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