An introduction to causality in quantum theory (and beyond)

V. Vilasini

Born on 15/10/1994,
Puducherry, India

Supervised by:
Dr. Lídia del Rio
Dr. Christopher Portmann
Prof. Renato Renner

A thesis submitted for the degree of
MSc. Physics

September 2017

ETH zürich

Quantum Information Theory Group
Institute for Theoretical Physics
ETH Zürich

Acknowledgements

This dissertation has been a great learning experience for me and Prof. Renato Renner's role in leading me to my research interests is crucial. I thank him for the gentle guidance and deep insights that have helped build my understanding of the subject and importantly, my first research paper. Lídia has been a constant presence in this process as a supervisor and a friend. I am thankful to her for the long and absorbing discussions about quantum foundations, her encouragement at moments of crisis and her critical inputs for our paper. I thank Christopher for proposing the interesting project on *Composable security in relativistic quantum cryptography*, for his guidance and inputs for our research paper and my Masters' thesis, that gave me a push in the right direction. The members of the Quantum Information Theory group have contributed significantly through the group seminars and discussions in keeping me up to date with latest research.

All this would have been impossible without the financial support from the ETH Masters Scholarship and the Inlaks Scholarship (Inlaks Shivdasani Foundation, India) in funding my Masters' programme, for I could have never made it to ETH otherwise.

Thanks are due to Nemanja for all his support and for accepting to be the first audience for many of my mock talks. Lastly, but importantly, my mother, Sujatha has been the inspiration behind my academic pursuits, impressing upon me at a young age that knowledge should be sought not merely as means to an end, but as an end in itself.

Abstract

This Masters thesis consists of two projects:

1. *Composable security in relativistic quantum cryptography*: The research carried out as part of the thesis on this topic lead to the original research paper [1]. An abstract of this is provided in the preface of this report and will not be discussed further in this report. We refer the reader to the original paper for further information in this regard.

2. *Causality in quantum theory and beyond*: This will be the topic of this report. It consists primarily of a review of quantum causality followed by an analysis of and discussion about two mathematical frameworks for studying quantum causality. Below, we give an abstract of what one will encounter in this report.

In the light of Bell's theorem [2] and its experimental, loophole-free tests [3–5], it has become clear that the classical understanding of causality (summarised in [6, 7]) does not provide satisfactory explanations of quantum experiments involving entangled systems [8]. This implies that the notion of cause that governs quantum systems is fundamentally different from that which governs classical systems, which has fuelled much research in the direction of generalizing classical causal models and causal discovery algorithms to ones [9–13].

Alternatively, a top-down approach for understanding quantum causality is to devise more general frameworks for causal structures that in particular include classical and quantum ones, and then narrow down the properties of quantum causal structures. For example, traditionally, one assumes a fixed background space-time structure while describing physical phenomena but recent approaches to modelling causal structures [14–18] within more general frameworks have shown that one can study cause-effect relations even without referring to an underlying space-time structure. In particular, violations of special relativity such as closed-timelike-curves (CTCs) do not arise even when such an assumption is dropped and it is possible to have causal structures that are themselves subject to fundamental quantum principles such as superposition and uncertainty and are not compatible with a definite causal order. Some indefinite causal structures of this kind may be seen to arise in situations where quantum mechanics and general relativity are jointly applied [19]: as Lucien Hardy pointed out in [15], general relativity is a deterministic theory without dynamic a causal structure that is dependent on the mass distribution while standard quantum theory is fundamentally indeterministic but has a fixed background causal structure. Thus a theory of quantum gravity should incorporate both these aspects.

There are a number of frameworks that model quantum causal structures [14–18] and in this report, we will review two of them: the causal boxes framework [18] and the process matrix framework [16]. While the process matrix framework models "superpositions of causal orders" in the absence of a global causal ordering (for example a fixed background space-time), the causal boxes framework shows us that the known, physically implementable examples (for instance, the quantum switch [20]) of such superpositions can be modelled within a fixed global ordering as well. This raises the question of whether these are really "superpositions of causal ordering" of space-time events or merely "superpositions of the temporal order" of operations. After reviewing the causal box and process matrix frameworks in detail and the representations of the quantum switch in these two frameworks, we compare the two representations and show that they are mathematically equivalent up to certain trivial factors. We then critically examine the different physical interpretations that could underlie this "mathematical equivalence" and proceed to discuss some of the similarities and differences in these frameworks. Lastly, we list some of the interesting open questions in this direction.

Preface

Here we provide an abstract of the first part of this masters thesis as it appears on the paper titled *Composable security in relativistic quantum cryptography* [1]. We refer the reader to the original paper for further information in this regard.

Relativistic protocols have been proposed to overcome some impossibility results in classical and quantum cryptography. In such a setting, one takes the location of honest players into account, and uses the fact that information cannot travel faster than the speed of light to limit the abilities of dishonest agents. For example, various relativistic bit commitment protocols have been proposed. Although it has been shown that bit commitment is sufficient to construct oblivious transfer and thus multiparty computation, composing specific relativistic protocols in this way is known to be insecure. A composable framework is required to perform such a modular security analysis of construction schemes, but no known frameworks can handle models of computation in Minkowski space. By instantiating the systems model from the Abstract Cryptography framework with causal boxes, we obtain such a composable framework, in which messages are assigned a location in Minkowski space (or superpositions thereof). This allows us to analyse relativistic protocols, and derive novel possibility and impossibility results. We show that (1) fair and unbiased coin flipping can be constructed from a simple resource called channel with delay; (2) biased coin flipping, bit commitment and channel with delay through any classical, quantum or post-quantum relativistic protocols are all impossible without further setup assumptions; (3) it is impossible to securely increase the delay of a channel, given several short-delay channels as ingredients. Results (1) and (3) imply in particular the non-composability of existing relativistic bit commitment and coin flipping protocols.

Please note that most of the original research carried out as part of this thesis are presented in the paper [1]. This report only covers the part of the thesis that is not presented in the paper. It consists primarily of a review of two frameworks (the causal box [18] and process matrix [16] frameworks) that can be used to study quantum causality, followed by a comparison of the two. The frameworks are quite different in their structure and applications, and to the best of our knowledge, such a systematic comparison of these two frameworks has not been carried out previously.

Contents

Chapter 1

Introduction

1.1 Classical causality

Deducing cause-effect relationships between random variables based on their observed statistical correlations has been crucial in diverse areas of science [6,7]; for example, in determining the effect of a certain drug in curing a disease and analysing the financial risks in a new undertaking, among others. Indeed it is common sense to expect that if physical variables are found to be statistically correlated, then this ought to have a causal explanation. However, correlations are symmetric while causal information is directional. To quote the example from [24]: "the statistical statement *the number of cars is correlated with the amount of air pollution* is different from the causal statement *cars cause air pollution.* The statistical statement goes both ways: Knowing there are more cars, one can infer that the air is more polluted and knowing the air is more polluted, one can infer that there are more cars. The causal statement tells us more; namely, if we change the number of cars, we can affect air pollution, but not vice versa: polluting the air by other means (say by building factories) will not affect the number of cars. Causal information is different from correlations because it tells us how the system changes under interventions."

One often hears "correlation does not imply causation". This is formalised by Reichenbach's principle [25] which states that if two variables are found to be correlated, then either one is a cause of the other or there is a third variable that is a common cause of both. "If an improbable coincidence has occurred, there must exist a common cause" he famously said. For example (Figure 1.1), if I observe that I get tired every time I go for a long run, this can be explained by the reasoning that the running causes me to expend energy which makes me tired i.e., running is a direct cause of my getting tired. On the other hand, if I observe that I tend to catch a cold on the days when the sales of room heaters peak, I would not conclude that rising room heater sales cause me to catch a cold or that my catching a cold causes room heater sales to rise but that a third factor, the cold weather is causing people to buy more room heaters and also causing me to fall sick. Here the cold weather is a common cause for both and given that the weather is cold, the correlations between my catching a cold and the room heater sales would disappear. If two correlated variables are found to have a common cause, the correlation will disappear if probabilities are conditioned to the common cause. In these simple examples, one was able to choose the most likely causal explanation simply through common sensical arguments, in most cases the causal explanation for the observed correlations is far from evident: if a researcher observes strong correlations between smoking and having cancer, should she conclude that smoking causes cancer, having cancer causes people to start smoking or that there exists a third, genetic factor which causes people to smoke and also increases their risk of cancer [13]? She would definitely not go for the second choice if it is found that getting cancer is often preceded (and not followed) by someone starting to smoke. In

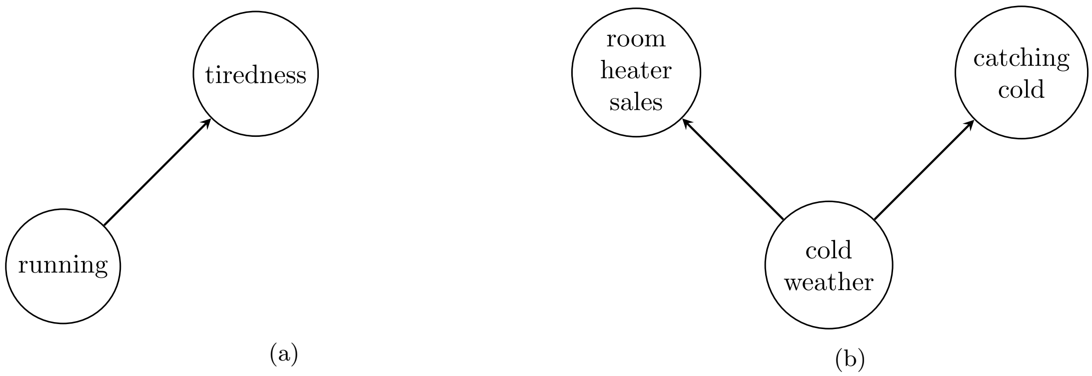


Figure 1.1: a) An example of a *directed acyclic graph* (DAG) representing a *direct cause* scenario. b) An example of a DAG representing a *common cause* scenario.

this case, the additional information about the temporal order of the events is known, which allows her to rule out one of the causal explanations because the effect cannot precede the cause. In the third case however, given that this genetic factor is present is enough to conclude that the person has a higher risk of cancer irrespective of whether or not he smokes and we can say that smoking and having cancer are conditionally independent given the genetic factor and smoking has no direct effect on cancer. Conditional independences provide new information about the statistical data and one needs to update their knowledge in the light of this new information, this is usually done through a process called Bayesian updating [6, 7]. The problem naturally gets more complex as the number of variables grow but these examples highlight that a model for describing cause-effect relations must take into account interventions as well as conditional dependences and a method for updating ones knowledge based on these independences.

Interventions, conditional independences and Bayesian updating based on these independences have been fairly well understood in the classical case and there are well established frameworks for classical causal models that take all these aspects into account [6, 7]. For the purpose of systematically deducing the causal relations between a set of variables from their observed statistical correlations, mathematical models for causal discovery have been extensively studied and we now have many causal discovery algorithms that serve the purpose (summaries in [6, 7] and the references therein).

1.2 Quantum Causality: Implications of Bell's theorem

Having invested a tremendous effort over the course of several years in understanding and building solid frameworks for modelling classical causality, it is natural to ask whether the same methods could be applied to deduce cause-effect relations between microscopic quantum systems. One finds that existing classical causal discovery algorithms (i.e., algorithms for deducing cause-effect relationships from statistical date) fail to satisfactorily explain quantum cause-effect relations [8]. This result is an unavoidable consequence of Bell's theorem [2]. In a loophole-free Bell experiment between Alice's and Bob, a direct cause relation between Alice and Bob's systems is ruled out by the non-signalling conditions. Reichenbach's principle [25] then implies that Alice's and Bob's systems share a common cause which could be a hidden variable in the joint causal past of the two systems. This means that the observed correlations between Alice's and Bob's systems must disappear when conditioned on this hidden variable which is their common cause. But a loophole-free Bell violation rules out exactly this: quantum correlations from entangled particles do not disappear even when conditioned on such hidden variables. This implies that the notion of cause that governs microscopic systems is fundamentally different, which has fuelled much research in quantum causal models [9–11] and quantum causal discovery [12, 13].

The work by John-Mark Allen et al. [9] provides a description of quantum common causes based on a quantum version of the Reichenbach principle that they generalise from a mathematical form of the original principle. They then use this notion of quantum common causes to build a basic quantum causal model that models interventions and conditional independences and provides a method for Bayesian updating. While this model comes a long way in providing a quantum definition of causation, many open questions still remain. For example, the work [9] provides an unambiguous way of understanding conditional independences in simple scenarios such as that of common cause, but a full understanding of quantum conditional independences in general scenarios with more interacting systems is still lacking.

1.3 More general causal structures

Another approach to studying causality is to devise general frameworks for causal structures that in particular include classical and quantum ones, and then try to narrow down the properties of quantum causal structures. This is a top-down approach as compared to the bottom-up approach of the previous section where one tries to build a quantum framework for modelling causal structures predicted by quantum experiments. The top-down approaches are the focus of this report.

fTraditionally, the assumption of a fixed background causal structure is often made while describing physical phenomena. However, recent approaches to modelling causal structures [14–18] within more general frameworks have shown that violations of special relativity such as *closed-timelike-curves* (CTCs) do not arise even when such an assumption is dropped. More specifically, it is possible to have causal structures that are themselves subject to fundamental quantum principles such as superposition and uncertainty. This opens up the interesting theoretical possibility of a large class of processes admitting no definite causal order, which are not in contradiction with any known laws of physics. These include processes involving superpositions of definite causal structures as well as more general processes which admit no causal explanation, not even as a superposition of fixed causal orders [16, 21, 22].

Some examples of indefinite causal structures may be seen to arise in hypothetical situations where quantum mechanics and general relativity are jointly applied. For example [19], if one considers a massive object in superposition at different spatial locations, the gravitational field produced by the object will also be in a superposition of different configurations (one corresponding to each spatial location of the object) and so will the space-time geometry itself. In such a scenario, the space-time metric does not have a definite value and it is not fixed in advance whether the space-time interval between two space-time points is space-like or time-like. In fact, it is believed that [15, 19] a complete theory of quantum gravity would have the indeterminism of quantum theory and the dynamic causal structures of general relativity, and that a correct and complete understanding of (space-)time and causality at the quantum level (which is currently lacking) would be crucial for overcoming some of the major difficulties in formulating such a unified theory.

It is not known whether processes without a causal explanation occur in nature; however, an example of a process that is claimed to implement a *superposition of causal orders* [21, 26] is the *quantum switch* [20]. The quantum switch, as its name suggests, switches between the order of two operations on a target system depending coherently on the value of a control system which is in a quantum superposition. This was physically implemented in [26, 27]. However, such processes still admit a causal explanation [18,21], and it can be debated whether the quantum switch implements a *superposition of causal orders* between two space-time events or merely a *superposition of temporal order* of two quantum operations (Section 4.1.3). Irrespective of the answer to this debate which would be of foundational importance, the quantum switch (discussed in Sections 1.4 and 4.1) is shown to provide a computational advantage over fixed ordering of operations for tackling certain

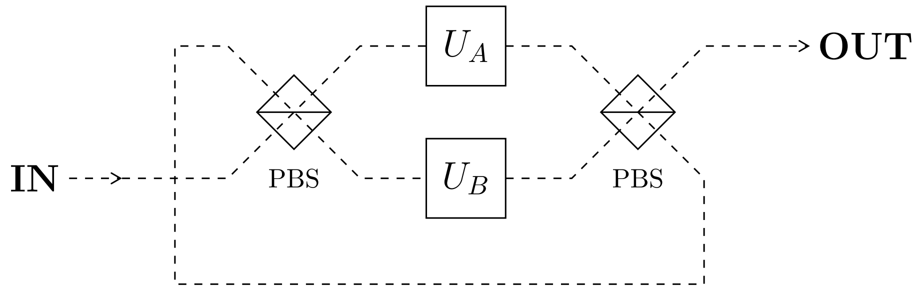


Figure 1.2: **Linear optical implementation of the quantum switch (Figure 1 [29]):** A horizontally polarized photon is transmitted by the all the polarizing beam splitters (PBSs) and takes the path where the unitary U_A is applied first and then U_B while a vertically polarized photon is reflected by all PBSs and follows the path where U_B is applied before U_A. The unitaries U_A and U_B act on internal degrees of freedom of a single photon other than its polarization state e.g., angular momentum modes. Thus the control and target states are encoded in different degrees of freedom of the same photon. [29]

operational tasks [28, 29]. Many existing frameworks such as that of quantum combs [30] and the quantum circuit model assume a fixed, pre-defined order of operations and do not capture the actual implementation [26, 27] of the quantum switch which involves a superposition of orders of quantum operations. This creates a need for frameworks that can model dynamic ordering of operations and superpositions thereof. Some examples of such frameworks are: the causaloid framework [15], the multi-time states formalism [14, 31, 32], the process matrix framework [16] and the causal box framework [18].

1.4 Superpositions of orders: the quantum switch

The quantum switch (QS) [20] is an example of a physically implementable [26, 27] process that cannot be described using a fixed, pre-defined order of operations, but requires a dynamic, quantum controlled ordering. The simplest quantum switch is a quantum process that coherently switches between the order or two operations depending on the value of a quantum control bit.

More formally, consider two qubit Hilbert spaces $\mathcal{H}^C$ and $\mathcal{H}^T$ where the former denotes the (pure) state space of the control qubit and the latter that of the target qubit. A quantum switch takes as input the state $(\alpha\,|0\rangle + \beta\,|1\rangle)_C \otimes |\Psi\rangle_T \in \mathcal{H}^C \otimes \mathcal{H}^T$ (with $|\alpha|^2 + |\beta|^2 = 1$) and outputs the state $(\alpha\,|0\rangle_C\, U_B U_A\,|\Psi\rangle_T + \beta\,|1\rangle_C\, U_A U_B\,|\Psi\rangle_T) \in \mathcal{H}^C \otimes \mathcal{H}^T$ where $|\Psi\rangle$ is an arbitrary qubit state in $\mathcal{H}^T$ and U_A, U_B are unitaries that act on the target qubit and represent the events A and B whose orders are switched by QS.

$$(\alpha\,|0\rangle + \beta\,|1\rangle)_C \otimes |\Psi\rangle_T \to \alpha\,|0\rangle_C \otimes U_B U_A\,|\Psi\rangle_T + \beta\,|1\rangle_C \otimes U_A U_B\,|\Psi\rangle_T \tag{1.1}$$

A schematic of the experimental setup used to realise this process is shown in Figure 1.2 which is adapted from [29]. Note that each of the unitaries U_A and U_B (given as black boxes) is queried only once. In fact this process cannot be represented as a regular quantum circuit if one requires that the unitaries U_A and U_B are queried only once each. If at least one unitary could be queried twice, then there is an almost trivial circuit representation as shown in Figure 1.3. In fact, the quantum switch was shown to have a computational advantage over fixed ordering of operations in solving certain computational tasks [28, 29] as it reduces the query complexity.

The quantum switch as implemented in [26, 27] i.e., with one query to each black-box unitary cannot be represented in the quantum circuit model, but there exist other, more general formalisms

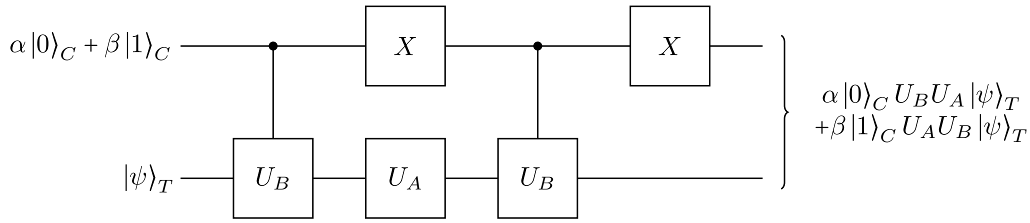


Figure 1.3: **Minimal circuit representation of the quantum switch:** To represent the quantum switch as a circuit, one needs to query at least one of the unitaries twice. Note that a controlled unitary (given as a black box) such as U_B in the figure can be implemented using controlled swaps between the control qubit, the target and an ancilla system (of the same dimensions as the target). In such a case, each of the unitaries U_A and U_B would be applied only once to the target but at least one of them would have been queried twice, where the additional query comes from the unitary acting on the ancilla system. However, the physical implementation of the quantum switch achieves the task with not more than one query to each unitary [26, 27]. This can be modelled using frameworks which do not assume a fixed ordering of operation, such as [14–16, 18, 32].

for modelling such processes with no definite causal order, such as the process matrix formalism [16] and causal boxes [18] among others [15].

1.5 Structure of this thesis

In this work, we review the causal box [18] and process matrix [16] frameworks in detail in Chapters 2 and 3 respectively. In Chapter 4 we compare the two frameworks. First, in Section 4.1, we review the description of the quantum switch in both formalisms and show that they are mathematically equivalent up to certain trivial factors. Following this, we critically examine the different physical interpretations that underlie this mathematical equivalence and in Section 4.2, we provide a systematic and detailed comparison of the two frameworks from a general perspective. Finally, we conclude with a summary of open questions in Section 4.3.

Chapter 2

The causal box framework [18]

The Causal Box [18] formalism models information-processing systems that are closed under composition. Similar formalisms have been previously developed but they are only suitable for modelling systems where the order of messages is predefined. An example of such a framework is that of *quantum combs* [30], similar formalisms were developed in [33, 34]). A *quantum comb* is an information-processing system (Figure 2.1 [18]) where each tooth of the comb corresponds to an input and output (possibly quantum) message and is associated with a node that represents an operation on the input message. The teeth of the comb define a fixed order on the operations and the quantum comb framework models these objects in a way that they can be described independently of their internal state and also provides rules for composing different combs when the order of messages is fixed. Thus the quantum combs framework cannot model situations where the causal structure is not predefined, e.g., when it is determined by a coin toss or coherently by the value of a quantum control bit. Indeed, consider a three-player protocol [18] where Alice and Bob send a random message to Charlie at different times and Charlie outputs the first message he receives and ignores the second. While the information processing tasks performed by Alice, Bob and Charlie separately can be described by individual quantum combs, the composition of the three systems is no longer a well-defined comb because it takes no input and produces one undetermined output (either Alice's or Bob's message, but it is not known in advance which one will be output by Charlie).

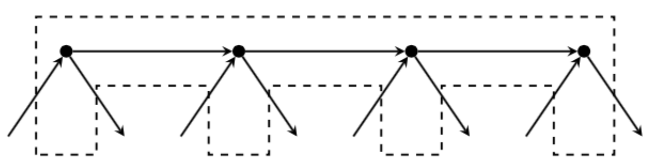


Figure 2.1: **An example of a quantum comb (Figure 1 [18], 2017 IEEE):** Each tooth of the comb corresponds to an input and output (possibly quantum) message and is associated with a node that represents an operation on the input message. The teeth of the comb define a fixed order on the operations.

When information processing systems are modelled as causal boxes, arbitrary composition of these systems is well defined even when the causal order is indefinite or dynamically determined during the protocol's runtime. Within the framework, a player can choose to send a message $|\Psi\rangle$ to another player or send nothing, which is denoted by the vacuum state $|\Omega\rangle$ or even a superposition

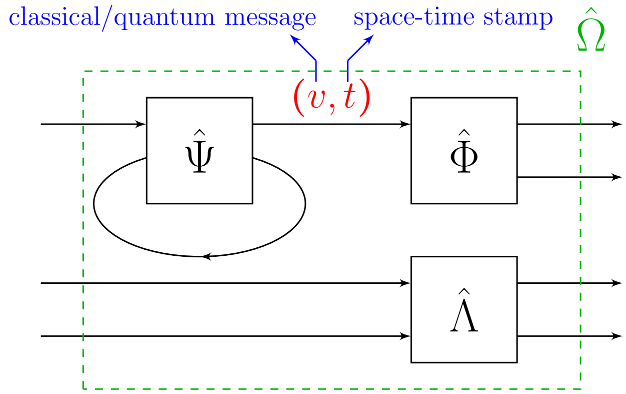


Figure 2.2: **Causal boxes (Figure 5a [1])** are information processing systems that respect causality and are closed under composition (serial, parallel or loops). Arbitrary composition of the causal boxes $\hat{\Phi}$, $\hat{\Psi}$ and $\hat{\Lambda}$ is a causal box $\hat{\Omega}$. Every message is modelled as a pair, (v, t) where v denotes the classical/quantum message and t provides ordering information and could be thought of as the space-time location at which the message is sent or received.

of the two i.e., a state of the form $\alpha |\Psi\rangle + \beta |\Omega\rangle$. A message could also be in a superposition of being sent to Alice and being sent to Bob i.e., in the state: $\alpha |\Psi\rangle_A \otimes |\Omega\rangle_B + \beta |\Omega\rangle_A \otimes |\Psi\rangle_B$. Thus players can exchange a superposition of different numbers of messages in a superposition of orders. Every output of a causal box can only depend on inputs ordered before it and hence the superposition of orders mentioned before corresponds to a superposition of causal structures, where each term of the superposition corresponds to a definite causal structure.

Such superpositions involving the vacuum state $|\Omega\rangle$ have been shown to be necessary for the physical realisation of information processing tasks such as controlling an unknown unitary [35]. The task involves applying an unknown unitary (given as a black box) on a target qubit only if the control qubit is in the state $|1\rangle$ and not applying any operation (i.e., performing an identity) otherwise. Interestingly, this task was initially proven to be impossible in theory [36, 37], yet it was realised experimentally [38]. The reason for this seemingly paradoxical situation is that the theoretical proof did not take into account the existence of a quantum state, $|\Omega\rangle$ that is invariant under the action of all unitaries i.e., $U|\Omega\rangle = |\Omega\rangle, \forall U$ while this is experimentally possible by sending "nothing" through a wire[1] as well as superpositions of sending "nothing" and "something". The impossibility proof does not go through in this case since one of the eigenvalues of the unknown unitary U is known (its action on $|\Omega\rangle$ is known).

2.1 Message space and wires

We now review the formal definitions of the objects of the causal box framework [18]. The main ingredients of the framework are the space of ordered quantum messages, input and output wires that can carry different numbers of such messages and a set of maps (which together describe a *causal box*) that obey causality and describe how the contents of the input wires transform into those at the outputs at different "times". The formalism then provides a method for combining or "composing" these maps in different ways to create a new set of maps (Figure 2.2).

1. **Space of ordered messages:** Every message is modelled as a pair, (v, t) where $v \in \mathcal{V}$

[1] A unitary acting on no input (i.e., the vacuum state $|\Omega\rangle$) produces no output and hence leaves the state invariant.

denotes the message and $t \in \mathcal{T}$ provides ordering information and could be thought of as the space-time location at which the message is sent or received where $\mathcal{T}$ is a countable, partially ordered set. The space of a single message is thus a Hilbert space with the orthonormal basis $\{|v,t\rangle\}_{v\in\mathcal{V},t\in\mathcal{T}}$. For a finite $\mathcal{V}$ and infinite $\mathcal{T}$, this Hilbert space corresponds to $\mathbb{C}^{|\mathcal{V}|} \otimes l^2(\mathcal{T})$ where $l^2(\mathcal{T})$ is the sequence space with a bounded 2-norm. For $|\mathcal{V}| = d > 2 \in \mathbb{N}$, this Hilbert space represents the state-space of a qudit with position[2] information. For example. the state $|\psi\rangle = \frac{1}{\sqrt{2}}(|0,t\rangle + |1,t\rangle) = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \otimes |t\rangle$ belongs to the space corresponding to a qubit with time information and corresponds to the qubit state $\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ being sent/received at time $t \in \mathcal{T}$.

2. **Wires:** The inputs and outputs to a causal box are sent/received through wires which can carry any number (or a superposition of different numbers) of messages of a fixed dimension, which defines the dimension of the wire. For example a 2 dimensional wire can carry any number of qubits, or can be in a superposition of carrying 2 and 3 qubits but cannot carry qutrits. Thus the state space of a wire is defined to be a symmetric Fock space. It is modelled as a Fock space to allow for superpositions of different numbers of messages and it is a symmetric Fock space since all ordering information associated with the arriving qudits is already contained in the label $t \in \mathcal{T}$ and given this label, there is no other ordering on the qudits. For the Hilbert space, $\mathcal{H} = \mathbb{C}^d \otimes l^2(\mathcal{T})$, the corresponding bosonic Fock space is given as
$$\mathcal{F}(\mathbb{C}^d \otimes l^2(\mathcal{T})) := \bigoplus_{n=0}^{\infty} \vee^n (\mathbb{C}^d \otimes l^2(\mathcal{T})), \tag{2.1}$$
where $\vee^n \mathcal{H}$ denotes the symmetric subspace of $\mathcal{H}^{\otimes n}$ and $\mathcal{H}^{\otimes 0}$ is the one-dimensional space containing the vacuum state $|\Omega\rangle$.

For example, the state space corresponding to a wire A carrying d_A dimensional messages is denoted by $\mathcal{F}_A^{\mathcal{T}} = \mathcal{F}(\mathbb{C}^{d_A} \otimes l^2(\mathcal{T}))$. The joint space of two wires can be written as $\mathcal{F}_A^{\mathcal{T}} \otimes \mathcal{F}_B^{\mathcal{T}} = \mathcal{F}_{AB}^{\mathcal{T}}$ and it can be shown [18] that for any two Hilbert spaces $\mathcal{H}_A = \mathbb{C}^{d_A} \otimes l^2(\mathcal{T})$ and $\mathcal{H}_B = \mathbb{C}^{d_B} \otimes l^2(\mathcal{T})$,
$$\mathcal{F}(\mathcal{H}_A) \otimes \mathcal{F}(\mathcal{H}_B) \cong \mathcal{F}(\mathcal{H}_A \oplus \mathcal{H}_B), \tag{2.2}$$
$$(\mathbb{C}^{d_A} \otimes l^2(\mathcal{T}) \oplus (\mathbb{C}^{d_B} \otimes l^2(\mathcal{T}) \cong (\mathbb{C}^{d_A} \oplus \mathbb{C}^{d_B}) \otimes l^2(\mathcal{T}). \tag{2.3}$$
Hence $\mathcal{F}_{AB}^{\mathcal{T}}$ can be interpreted as the state space of a wire carrying $(d_A + d_B)$ dimensional messages. Conversely, any wire A of messages of dimension d_A can be split in two sub-wires A_1 and A_2 of messages of dimensions $d_{A_1} + d_{A_2} = d_A$:
$$\mathcal{F}_A^{\mathcal{T}} \cong \mathcal{F}_{A_1}^{\mathcal{T}} \otimes \mathcal{F}_{A_2}^{\mathcal{T}}. \tag{2.4}$$
Further, for any subset $\mathcal{P} \subseteq \mathcal{T}$,
$$\mathcal{F}_A^{\mathcal{T}} \cong \mathcal{F}_A^{\mathcal{P}} \otimes \mathcal{F}_A^{\widetilde{\mathcal{P}}}, \tag{2.5}$$
where $\widetilde{\mathcal{P}} = \mathcal{T} \backslash \mathcal{P}$ and $\mathcal{F}_A^{\mathcal{P}} = \mathbb{C}^{d_A} \otimes l^2(\mathcal{P})$.

An example at this point would be illustrative. An orthonormal basis for the Hilbert space of a single message encoded in a qubit is given by $\mathcal{H}_{qb} = \{|(i,t)\rangle_{i\in\{0,1\},t\in\mathcal{T}}\}$. The basis for $\mathcal{H}_{qb}^{\otimes 2}$ is then given by $\{|(i_1,t_1),(i_2,t_2)\rangle\}_{i_1,i_2\in\{0,1\},t_1,t_2\in\mathcal{T}}$ and $\mathcal{H}_{qb}^{\vee^2}$ which is the symmetric subspace of $\mathcal{H}_{qb}^{\otimes 2}$ is denoted by
$$\vee\, \mathrm{span}(\{|(i_1,t_1),(i_2,t_2)\rangle_{i_1,i_2\in\{0,1\},t_1,t_2\in\mathcal{T}}\}).$$

[2] $\mathcal{T}$ is modelled as a partially ordered set in the framework, this could physically correspond to space-time or simply time information depending on the situation. We will often refer to this as "position" information.

Now a state in $\mathcal{H}_{qb}^{\vee^2}$ corresponding to the message 0 being sent at time t_1 and the message 1 being sent at time t_2 which we can denote in short-hand by $|\text{“}(0,t_1),(1,t_2)\text{”}\rangle := |\text{“}01\text{”}\rangle$, represents the symmetric state given in Equation (2.6a). Similarly the state corresponding to 1 being sent at t_1 and 0 at t_2 can be denoted as $|\text{“}(1,t_1),(0,t_2)\text{”}\rangle := |\text{“}10\text{”}\rangle$ and represents the symmetric state given in Equation (2.6b). The reason for the symmetrisation is now more apparent: there is no physical different between the states $|\text{“}(0,t_1),(1,t_2)\text{”}\rangle$ and $|\text{“}(1,t_2),(0,t_1)\text{”}\rangle$ since all the ordering information corresponding to the messages is already contained in their respective position labels t_1 and t_2.

$$|\text{“}01\text{”}\rangle = \frac{1}{\sqrt{2}}(|0,t_1\rangle \otimes |1,t_2\rangle + |1,t_2\rangle \otimes |0,t_1\rangle), \tag{2.6a}$$

$$|\text{“}10\text{”}\rangle = \frac{1}{\sqrt{2}}(|1,t_1\rangle \otimes |0,t_2\rangle + |0,t_2\rangle \otimes |1,t_1\rangle) \tag{2.6b}$$

An analogue of the maximally entangled, singlet state in this space can be written as follows. Note that this is still a symmetric state belonging to $\mathcal{H}_{qb}^{\vee^2}$.

$$\frac{1}{\sqrt{2}}(|\text{“}01\text{”}\rangle - |\text{“}10\text{”}\rangle) = \frac{1}{\sqrt{2}}(|0,t_1\rangle \otimes |1,t_2\rangle + |1,t_2\rangle \otimes |0,t_1\rangle - |1,t_1\rangle \otimes |0,t_2\rangle - |0,t_2\rangle \otimes |1,t_1\rangle) \tag{2.7}$$

Now we can see how Equation (2.2) comes about. Consider two wires A and B. The state spaces of these wires are denoted as $\mathcal{F}(\mathcal{H}_A) := \mathcal{F}_A$ and $\mathcal{F}(\mathcal{H}_B) := \mathcal{F}_B$ respectively. Let $\{|(u,t)\rangle\}_{u\in\mathcal{U},t\in\mathcal{T}}$ and $\{|(v,t)\rangle\}_{v\in\mathcal{V},t\in\mathcal{T}}$ be a orthonormal bases of $\mathcal{H}_A$ and $\mathcal{H}_B$. The orthonormal basis of $\mathcal{H}_A^{\otimes 2}$ is then denoted by $\{|(u_1,t_1),(u_2,t_2)\rangle\}_{u_1,u_2\in\mathcal{U},t_1,t_2\in\mathcal{T}}$ and similarly for higher order tensor products of $\mathcal{H}_A$ and $\mathcal{H}_B$. The corresponding Fock spaces can then be written as follows:

$$\mathcal{F}(\mathcal{H}_A) = \vee\,\text{span}\{ \overbrace{\{\}}^{\text{no messages}}, \overbrace{\{|(u,t)\rangle\}_{u\in\mathcal{U},t\in\mathcal{T}}}^{\text{1 message}}, \overbrace{\{|(u_1,t_1),(u_2,t_2)\rangle\}_{u_1,u_2\in\mathcal{U},t_1,t_2\in\mathcal{T}}}^{\text{2 messages}}, ...\}, \tag{2.8a}$$

$$\mathcal{F}(\mathcal{H}_B) = \vee\,\text{span}\{ \overbrace{\{\}}^{\text{no messages}}, \overbrace{\{|(v,t)\rangle\}_{v\in\mathcal{V},t\in\mathcal{T}}}^{\text{1 message}}, \overbrace{\{|(v_1,t_1),(v_2,t_2)\rangle\}_{v_1,v_2\in\mathcal{V},t_1,t_2\in\mathcal{T}}}^{\text{2 messages}}, ...\}, \tag{2.8b}$$

where $\vee span\{|i\rangle\}_{i\in\mathcal{I}}$ is the symmetric subspace of the span of the orthonormal basis $\{|i\rangle\}_{i\in\mathcal{I}}$ and the set $\{\}$ denotes the “no message”, i.e., the vacuum state, which being the only state in $\mathcal{H}^{\otimes 0}$ is also the orthonormal basis for this Hilbert space. From the above equations, we can write a similar equation for the tensor product of the two Fock spaces[3].

$$\begin{aligned} \mathcal{F}(\mathcal{H}_A) \otimes \mathcal{F}(\mathcal{H}_B) = \vee span\{ &\overbrace{\{\{\},\{\}\}}^{\text{0 messages}}, \overbrace{\{\{|(u,t)\rangle\},\{|(v,t)\rangle\}\}}^{\text{1 message}}, \\ &\overbrace{\underbrace{\{\{|(u_1,t_1),(u_2,t_2)\rangle\}}_{\text{2 in A, 0 in B}}, \underbrace{\{|(v_1,t_1),(v_2,t_2)\rangle\}}_{\text{0 in A, 2 in B}}, \underbrace{\{|(u_1,t_1),(v_2,t_2)\rangle\},\{|(v_1,t_1),(u_2,t_2)\rangle\}\}}_{\text{1 in A, 1 in B}}}^{\text{2 messages}}, ...\} \end{aligned} \tag{2.9}$$

Relabelling the terms in the following manner then gives the desired isomorphism: Equation (2.2).

$$\overbrace{\{\{\},\{\}\}}^{\text{0 messages}} \longrightarrow \overbrace{\{\}}^{\text{0 messages}}$$

[3]We drop the subscripts in the basis sets for convenience, but it must be understood that $u,u_1,u_2 \in \mathcal{U}, v, v_1, v_2 \in \mathcal{V}, t, t_1, t_2 \in \mathcal{T}$.

$$\overbrace{\{\{|(u,t)\rangle\},\{|(v,t)\rangle\}\}}^{\text{1 message}} \longrightarrow \overbrace{\{|(w,t)\rangle\}_{w\in\mathcal{U}\cup\mathcal{V},t\in\mathcal{T}}}^{\text{1 message}}$$

$$\overbrace{\{\underbrace{\{|(u_1,t_1),(u_2,t_2)\rangle\}}_{\text{2 in A, 0 in B}}, \underbrace{\ldots}_{\text{0 in A, 2 in B}}, \underbrace{\ldots}_{\text{1 in A, 1 on B}}\}}^{\text{2 messages}} \longrightarrow \overbrace{\{|(w_1,t_1),(w_2,t_2)\rangle\}_{w_1,w_2\in\mathcal{U}\cup\mathcal{V},t_1,t_2\in\mathcal{T}}}^{\text{2 messages}}$$

$$\mathcal{F}(\mathcal{H}_A)\otimes\mathcal{F}(\mathcal{H}_B) \cong \{ \overbrace{\{\}}^{\text{0 messages}}, \overbrace{\{|(w,t)\rangle\}_{w\in\mathcal{U}\cup\mathcal{V},t\in\mathcal{T}}}^{\text{1 message}}, \tag{2.10}$$

$$\overbrace{\{|(w_1,t_1),(w_2,t_2)\rangle\}_{w_1,w_2\in\mathcal{U}\cup\mathcal{V},t_1,t_2\in\mathcal{T}}}^{\text{2 messages}}, \ldots\ldots\} = \mathcal{F}(\mathcal{H}_A\oplus\mathcal{H}_B) \tag{2.11}$$

The isomorphism tells us that each valid state in the combined state space of two wires, one carrying d_A dimensional messages and the other carrying d_B dimensional messages, can be mapped to a valid state in the state space of a single wire carrying $d_A + d_B$ dimensional messages. Although the isomorphism follows from a trivial mathematical relabelling as shown above, the states related by the isomorphism would physically correspond to different preparation procedures. Again, an example would be illustrative.

We noted in the previous example that the "singlet" state in Equation (2.7) is still a symmetric state belonging to $\mathcal{H}_{qb}^{\vee^2}$. More generally, this could be thought of as a state in $\mathcal{F}(\mathcal{H}_{qb})$ i.e., the state space of a wire carrying 2 dimensional messages (encoded in qubits). Note that setting $t_1 = t_2 = t$ in Equation (2.7) reduces the state to 0. This is because for $t_1 = t_2 = t$, the two terms appearing in the superposition are physically the same (there is no ordering information coming from the position label) and they cancel out: both terms correspond to sending the messages 0 and 1 at time t. This is natural since the singlet state of two qubits is an anti-symmetric state in the 2-qubit state space and the symmetric subspace of 2-qubits is the 3 dimensional subspace spanned by the vectors $\{|00\rangle,|11\rangle,\frac{1}{\sqrt{2}}(|01\rangle+|10\rangle)\}$. Thus a 2 dimensional wire with state space $\mathcal{F}(\mathcal{H}_{qb})$ can only carry messages $u\in\mathcal{U}=\mathrm{span}(\{|00\rangle,|11\rangle,\frac{1}{\sqrt{2}}(|01\rangle+|10\rangle)\})$. If we want to send the message $\frac{1}{\sqrt{2}}(|01\rangle-|10\rangle)\}$ i.e., the singlet state at time t, we could either send it as a single message through a wire that can carry 4 dimensional messages or by virtue of the isomorphism of Equation (2.2), we could encode it into two 2 dimensional wires. In particular, we can have the following scenarios:

1. Consider a single message $v=\frac{1}{\sqrt{2}}(|01\rangle-|10\rangle)$ sent through a 4 dimensional wire at time t (with basis $\{|(v,t)\rangle\}_{v\in\mathcal{V},t\in\mathcal{T}}$, $\mathcal{V}=\{00,01,10,11\}$). Using the isomorphism, this could be encoded in two wires such that the first bit of a label 01 denotes the wire and the second bit denotes the value. Hence $\frac{1}{\sqrt{2}}(|(01,t)\rangle-|(10,t)\rangle)$ would be an equal superposition of sending the qubit state $|1\rangle$ on wire 0 and the state $|0\rangle$ on wire 1, both at time t. Note that for the single 4 dimensional wire, the state is not entangled in this case since the basis labels $\{00,01,10,11\}$ could simply be relabelled as $\{0,1,2,3\}$ and the message simply becomes $v=\frac{1}{\sqrt{2}}(|1\rangle-|2\rangle)$ sent at time t.

2. An entangled state for the 4 dimensional wire would require at least two (4D) messages, for example one can consider the state $\frac{1}{\sqrt{2}}(|\text{“}(0,t),(3,t)\text{”}\rangle-|\text{“}(1,t),(2,t)\text{”}\rangle)=\frac{1}{\sqrt{2}}(|\text{“}(00,t),(11,t)\text{”}\rangle-|\text{“}(01,t),(10,t)\text{”}\rangle)$ where $|\text{“}(x),(y)\text{”}\rangle=\frac{1}{\sqrt{2}}(|(x),(y)\rangle+|(y),(x)\rangle)$. By the same isomorphism, this can be encoded into two 2 dimensional wires (labelled by 0 and 1) as a superposition of "*send* $|0\rangle$ *through wire 0 and* $|1\rangle$ *through wire 1 at time* t" and "*send* $|1\rangle$ *through wire 0 and* $|0\rangle$ *through wire 1 at time* t".

Having defined the input and output spaces of a causal box, a causal box can intuitively be thought of as a set of mutually consistent maps from inputs received at a certain set of positions to outputs produced at strictly later positions. In general, it is modelled as a set of maps and not a single map because this allows systems to be included which produce an unbounded number of messages and are thus not well-defined as a single map on the entire set $\mathcal{T}$, but only on subsets of $\mathcal{T}$ that are upper bounded by a set of unordered points. For example [18], a system that outputs a state $|0\rangle$ at every point $t \in \mathbb{N}$ is well-defined on every subset $\{1, ..., t\}$, but the limit behavior is not, as it would correspond to a box that outputs an infinite tensor product of $|0\rangle$.

Each map from the set characterising a causal box could be thought of as the map implemented when the causal box is allowed to produce outputs until positions that are no later than a set of unordered points. Naturally is is expected that the different maps characterising the same causal box are mutually consistent i.e., any two maps would give the same description of the causal box when restricted to the same set of positions. For a causal box where the set $\mathcal{T} = \{1, 2, 3, ...\}$ represents a time parameter, the set of maps would describe how the causal box would act on inputs if it is allowed to produce outputs until time $t = 1$, $t = 2$ and so on. Mutual consistency of maps would require that if one is asked to describe how the box behaves if it can produce outputs until $t = 5$, all the maps terminating at $t = 5$ or later should give the same answer i.e., tracing out outputs produced at position $t = 6$ to $t = N$ from a map from the set that produces outputs until $t = N$ should yield the map that stops producing outputs at $t = 5$.This will become clearer once we formally define a causal box in the following sections. But before we do so, we must first define cuts of a partially ordered set to formalise the meaning of upper-bounding by a set of points and make precise the notion of causality that would be invoked in the definition of a causal box.

2.2 Cuts and causality

Definition 2.2.1 (Cuts [18])**.** *A cut of a partially ordered set $\mathcal{T}$ is any subset $\mathcal{C} \subseteq \mathcal{T}$ such that*

$$\mathcal{C} = \bigcup_{t \in \mathcal{C}} \mathcal{T}^{\leq t},$$

where $\mathcal{T} \leq t = \{p \in \mathcal{T} : p \leq t\}$. A cut $\mathcal{C}$ is bounded *if there exists a point $t \in \mathcal{T}$ such that $\mathcal{C} \subseteq \mathcal{T}^{\leq t}$. The set of all cuts of $\mathcal{T}$ is denoted as $\mathfrak{C}(\mathcal{T})$ and the set of all bounded cuts as $\overline{\mathfrak{C}}(\mathcal{T})$.*

The definition is illustrated in Figures 2.3 and 2.4. If there is an arrow from a point $t \in \mathcal{T}$ to a point $t' \in \mathcal{T}$, then we can write $t \prec t'$ i.e., t' is in the "future" of t. The restriction to bounded cuts is justified if one is only interested in points along single "branches" (sets of points that have at least one point in their common future) i.e., one only cares about points that share a common "future" (Figure 2.3). Minkowski space-time is a particular candidate for the partially ordered set $\mathcal{T}$, where all possible cuts are necessarily bounded since any two space-time points (even those that are unordered i.e., space-like separated) necessarily share a common causal future. This need not be the case for a general partially ordered set $\mathcal{T}$, as seen in Figure 2.3. The different branches in such sets that share no common "future" are like different non-interacting universes and quantum mechanics on such spaces would in principle allow for quantum states to be copied into different branches without violating the no-cloning principle, since both copies can never be compared/accessed at the same position. However, it is enough to consider bounded cuts as they capture all known physical situations.

The causality criterion that "*an output can only depend on past inputs*" is formalised by requiring that for every causal box there exist a monotone function on the set of all cuts, $\chi : \mathfrak{C}(\mathcal{T}) \to \mathfrak{C}(\mathcal{T})$ such that an output on $\mathcal{C} \in \overline{\mathfrak{C}}(\mathcal{T})$ can be computed from the input on $\chi(\mathcal{C}) \subset \mathcal{C}$. The causality function is defined on cuts since in general, inputs generated at a set of unordered positions $\{t\}_{t \in \mathcal{T}}$ may be required to compute an output in their joint "future" $p \succ \{t\}_{t \in \mathcal{T}}$.

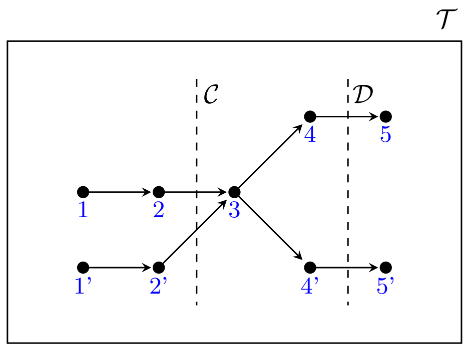


Figure 2.3: **Bounded and unbounded cuts on a partially ordered set:** In this example, the partially ordered set $\mathcal{T}$ contains 9 points. The cut $\mathcal{C} \in \overline{\mathfrak{C}}(\mathcal{T})$ is a bounded cut as all the points included in this cut, $1, 2, 1', 2'$ are all upper bounded by the single point 3 and their joint future is described by the set of points $\{3, 4, 5, 4', 5'\}$ which is non-empty. The cut $\mathcal{D} \in \mathfrak{C}(\mathcal{T})$ on the other hand is unbounded since the points 4 and $4'$ have no point in their joint future, they belong to different "branches" (sets of points that have at least one point in their common future). For example, 4 belongs to the branch given by the set of points $1, 2, 3, 4, 5$ while $4'$ belongs to the different branch given by the set $1, 2, 3, 4', 5'$ which does not include 4. The cuts are such that $\mathcal{C} \subset \mathcal{D}$ and include 4 and 7 points respectively.

Since the output on $\mathcal{C} \cup \mathcal{D}$ can be computed from $\chi(\mathcal{C}) \cup \chi(\mathcal{D})$ if the output on $\mathcal{C}$ can be computed from $\chi(\mathcal{C})$ and the output on $\mathcal{D}$ computed from $\chi(\mathcal{D})$, it is required that $\chi(\mathcal{C} \cup \mathcal{D}) = \chi(\mathcal{C}) \cup \chi(\mathcal{D})$. In addition, if $\mathcal{C} \subseteq \mathcal{D}$, then $\chi(\mathcal{C}) \subseteq \chi(\mathcal{D})$, because if $\chi(\mathcal{C})$ is needed to compute the output on $\mathcal{C}$, then certainly it is needed to compute the output on $\mathcal{D} \supseteq \mathcal{C}$.

Further, an additional condition is required to ensure that a causal box does not produce an infinite number of messages in a finite interval of time, for such an operation would be ill-defined. This could happen for example if the time gap between subsequent outputs of a system get smaller and smaller and the sequence of the gaps converges to zero. To quote a more concrete example from [18]: A system with $\mathcal{T} = \mathbb{Q}^{+}$, that for every input received in position $1 - t$, for $0 < t \leq 1, t \in \mathcal{T}$, produces an output in position $1 - t/2$ will have the causality function $\chi([0, 1 - t/2]) = [0, 1 - t]$. If this system initially outputs a message in position 0 and the messages output are looped back to the input, this system should produce messages at points $\{0, 1/2, 3/4, 7/8, 15/16, ...\}$ and thus the system produces an infinite number of messages before $t = 1$. Such situations are avoided by requiring that the causality function satisfies: $\forall \mathcal{C} \in \overline{\mathfrak{C}}(\mathcal{T}), \forall t \in \mathcal{C}, \exists n \in N\mathbb{N}, t \notin \chi^{n}(\mathcal{C})$. This can be easily seen by considering a cut $\mathcal{C}$ that includes the point $t = 1$. Any such cut would also include all points $t < 1$. Now all the points $t \in \{0, 1/2, 3/4, 7/8, 15/16, ...\}$ are "infinite" steps away from the point $t = 1$ since by construction the sequence converges to 1 and the causality function applied to $t = 1$ remains stuck at the same value which implies that these points will lie within the cut $\chi^{n}(\mathcal{C})$ for all $n \in \mathbb{N}$ which violates the new requirement. This condition is further explained in Figure 2.4. Putting these conditions together, the causality function is formally defined as follows:

Definition 2.2.2 (Causality function [18])**.** *A function* $\chi : \mathfrak{C}(\mathcal{T}) \to \mathfrak{C}(\mathcal{T})$ *is a* causality function *if it satisfies the following conditions:*

$$\forall \mathcal{C}, \mathcal{D} \in \mathfrak{C}(\mathcal{T}), \quad \chi(\mathcal{C} \cup \mathcal{D}) = \chi(\mathcal{C}) \cup \chi(\mathcal{D}), \tag{2.12a}$$

$$\forall \mathcal{C}, \mathcal{D} \in \mathfrak{C}(\mathcal{T}), \quad \mathcal{C} \subseteq \mathcal{D} \Rightarrow \chi(\mathcal{C}) \subseteq \chi(\mathcal{D}), \tag{2.12b}$$

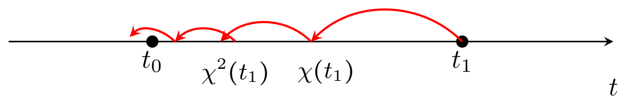


Figure 2.4: **Causality function:** Consider the totally ordered, 1 dimensional set $\mathcal{T} = \mathbb{R}^+$ as shown. The cut upper bounded by the point t_1 is now the set $\mathcal{T}^{\leq t_1} = \{p \in \mathcal{T} : p \leq t_1 \in \mathcal{T}\}$. The last condition [18] in Definition 2.2.2 ensures that any point $t_0 \prec t_1$ can be crossed from t_1 in a finite number of steps, where each "step" denotes one use of the causality function. In the above figure, t_0 is crossed in 4 steps and the cuts (in this case linear sets) $\chi^n(t)$ with $n \geq 4$ will not include the point t_0. The condition ensures that the causality function does not get "stuck" around any position as was the case with the example function $\chi([0, 1 - t/2]) = [0, 1 - t]$ seen in this section.

$$\forall \mathcal{C} \in \overline{\mathfrak{C}}(\mathcal{T}) \backslash \{\varnothing\}, \quad \chi(\mathcal{C}) \subset \mathcal{C}, \tag{2.12c}$$

$$\forall \mathcal{C} \in \overline{\mathfrak{C}}(\mathcal{T}), \forall t \in \mathcal{C}, \exists n \in \mathbb{N}, \quad t \notin \chi^n(\mathcal{C}), \tag{2.12d}$$

where χ^n denotes n compositions of χ with itself, $\chi^n = \chi \circ \cdots \circ \chi$.

Definition 2.2.2 is the general definition of the causality function and it simplifies for special choices of the set $\mathcal{T}$, as will be seen in Section 2.6. We are now in a position to review the formal definition of a causal box.

2.3 General definition of a causal box

Definition 2.3.1 (Causal box [18])**.** *A (d_X, d_Y)-causal box Φ is a system with input wire X and output wire Y of dimension d_X and d_Y[4], defined by a set of mutually consistent (Equation (2.14)), completely positive, trace-preserving (CPTP) maps (Equation (2.13))*

$$\Phi = \{\Phi^{\mathcal{C}} : \mathfrak{T}(\mathcal{F}_X^{\chi(\mathcal{C})}) \to \mathfrak{T}(\mathcal{F}_Y^{\mathcal{C}})\}_{\mathcal{C} \in \overline{\mathfrak{C}}(\mathcal{T})}. \tag{2.13}$$

These maps much be such that for all $\mathcal{C}, \mathcal{D} \in \overline{\mathfrak{C}}(\mathcal{T})$ with $\mathcal{C} \subseteq \mathcal{D}$,

$$tr_{\mathcal{D} \backslash \mathcal{C}} \circ \Phi^{\mathcal{D}} = \Phi^{\mathcal{C}} \circ tr_{\mathcal{T} \backslash \chi(\mathcal{C})}, \tag{2.14}$$

where $\mathfrak{T}(\mathcal{F})$ denotes the set of all trace class operators on the space $\mathcal{F}$ and the causality function $\chi(.)$ satisfies all the conditions of Definition 2.2.2. $\mathcal{F}^{\mathcal{C}}$ is the subspace of $\mathcal{F}^{\mathcal{T}}$ that contains only messages in positions $t \in \mathcal{C} \subseteq T$ and $tr_{\mathcal{D} \backslash \mathcal{C}}$ traces out the messages occurring at positions in $\mathcal{D} \backslash \mathcal{C}$.

Equation (2.14) can be seen as the combination of the two requirements $\Phi^{\mathcal{C}} = tr_{\mathcal{D} \backslash \mathcal{C}} \circ \Phi^{\mathcal{D}}$ and $\Phi^{\mathcal{C}} = \Phi^{\mathcal{C}} \circ tr_{\mathcal{T} \backslash \chi(\mathcal{C})}$. The first one embodies the mutual consistency requirement while the second, that of causality. $\Phi^{\mathcal{C}} = tr_{\mathcal{D} \backslash \mathcal{C}} \circ \Phi^{\mathcal{D}}$ says that a system producing outputs only at positions in $\mathcal{C}$ is obtained from a system producing outputs only at positions in $\mathcal{D} \supseteq \mathcal{C}$ by tracing out messages produced at positions in $\mathcal{D}$ that are not in $\mathcal{C}$. This ensures that two maps belonging to a set describing the same causal box are same when they are restricted to producing outputs within the same cut and hence describe the causal box consistently. $\Phi^{\mathcal{C}} = \Phi^{\mathcal{C}} \circ tr_{\mathcal{T} \backslash \chi(\mathcal{C})}$ says that only the inputs on positions $\chi(\mathcal{C}) \subset \mathcal{C}$ are relevant for computing the outputs on positions in $\mathcal{C}$, i.e., the output on $\mathcal{C}$ can only depend on inputs that are before, namely $\chi(\mathcal{C})$.

[4] It is enough to define a causal box as a map from one input wire to one output wire since a single wire of dimension d can always be decomposed into n wires of dimensions $d_1, ..., d_n$ with $d = d_1 + d_2 + ... + d_n$ using the isomorphism of Equation(2.2)

Note that Definition 2.3.1 only considers trace-preserving causal boxes. The definition can be easily generalised to non-trace preserving causal boxes or *sub-normalised causal boxes* to account for post-selection. This is done in [18] by defining a suitable projector on the space of *normalised causal boxes*. We will not go into the details of this definition here.

2.4 Representations of causal boxes

2.4.1 Choi-Jamiołkowski (CJ) representation

CJ representation for infinite dimensional Hilbert spaces: For finite dimensional Hilbert spaces $\mathcal{H}_A$ and $\mathcal{H}_B$, a CPTP map $\Phi : \mathcal{L}(\mathcal{H}_A) \to \mathcal{L}(\mathcal{H}_B)$ between the set of linear operators on the spaces has a Choi-Jamiołkowski (CJ) representation given by the positive, semi-definite Choi operator $R_\Phi \in \mathcal{L}(\mathcal{H}_{BA})$ defined as

$$R_\Phi = \sum_{i,j} \Phi(|i\rangle\langle j|) \otimes |i\rangle\langle j|, \tag{2.15}$$

satisfying,

$$tr_B R_\Phi = I_A. \tag{2.16}$$

Any positive semi-definite operator satisfying Equation (2.16) is the Choi-Jamiołkowski representation of some CPTP map. For infinite dimensional Hilbert spaces $\mathcal{H}_A$ and $\mathcal{H}_B$ however, the Choi operator of a map $\Phi : \mathfrak{T}(\mathcal{H}_A) \to \mathfrak{T}(\mathcal{H}_B)$ is often unbounded and the CJ representation needs to be defined slightly differently. In this case, the CJ representation is defined instead as the sesquilinear positive semi-definite form R_Φ on $\mathcal{H}_B \times \mathcal{H}_A = \text{span}\{\psi_B \otimes \psi_A : \psi_B \in \mathcal{H}_B, \psi_A \in \mathcal{H}_A\}$ that satisfies:

$$R_\Phi(\psi_B \otimes \psi_A; \phi_B \otimes \phi_A) \coloneqq \langle\psi_B| \Phi(|\overline{\psi_A}\rangle\langle\overline{\phi_A}|)|\phi_B\rangle, \tag{2.17}$$

where $|\overline{\psi}\rangle = \sum_{i=1}^{\infty} |i\rangle \overline{\langle i|\psi\rangle}$ represents complex conjugation in some fixed basis $\{|i\rangle_i\}$ of $\mathcal{H}_A$ (ref).

In the case that the operator corresponding to the sesquilinear form R_Φ is bounded, which happens when the corresponding Hilbert spaces are finite or when the domain of the form is all of $\mathcal{H}_B \otimes \mathcal{H}_A$, the operator $\hat{R_\Phi} \in \mathfrak{B}(\mathcal{H}_{BA})$ can be recovered as follows:

$$\langle\psi_B| \otimes \langle\psi_A| \hat{R_\Phi} |\phi_B\rangle \otimes |\phi_A\rangle = R_\Phi(\psi_B \otimes \psi_A; \phi_B \otimes \phi_A), \tag{2.18}$$

where the trace condition of Equation (2.16) becomes for any basis $\{|j\rangle\}_j$ of $\mathcal{H}_B$

$$\sum_j R_\Phi(i_B \otimes \psi_A; j_B \otimes \phi_A) = \langle\psi_A|\phi_A\rangle. \tag{2.19}$$

Analogous to the finite case, any positive semi-definite sesquilinear form satisfying Equation (2.19) uniquely defines a CPTP map $\Phi : \mathfrak{T}(\mathcal{H}_A) \to \mathfrak{T}(\mathcal{H}_B)$ [18]. CP but non-TP maps in finite case satisfy Equation (2.15) but not Equation (2.16), similar CP but non-TP maps in the infinite case satisfy Equation (2.17) but not Equation(2.19).

CJ representation of a causal box ([18], 2017 IEEE): A causal box, $\Phi = \{\Phi^{\mathcal{C}} : \mathfrak{T}(\mathcal{F}_X^{\chi(\mathcal{C})}) \to \mathfrak{T}(\mathcal{F}_Y^{\mathcal{C}})\}_{\mathcal{C} \in \overline{\mathfrak{C}}(\mathcal{T})}$ satisfying Definition 2.3.1 can be equivalently represented by the set of positive semi-definite sesquilinear forms $R_\Phi^{\mathcal{C}}$ that satisfy the following condition:

For any states $\psi_X^{\chi(\mathcal{C})}, \phi_X^{\chi(\mathcal{C})} \in \mathcal{F}_X^{\chi(\mathcal{C})}$, $\psi_X^{\widetilde{\chi(\mathcal{C})}}, \phi_X^{\widetilde{\chi(\mathcal{C})}} \in \mathcal{F}_X^{\widetilde{\chi(\mathcal{C})}}$, $\psi_Y^{\mathcal{C}}, \phi_Y^{\mathcal{C}} \in \mathcal{F}_Y^{\mathcal{C}}$ *and any basis* $\{|j\rangle_j\}$ *of*

$\mathcal{F}_Y^{\widetilde{\mathcal{C}}}$ *where* $\mathcal{F}_X^{\chi(\mathcal{D})} \cong \mathcal{F}_X^{\chi(\mathcal{C})} \otimes \mathcal{F}_X^{\widetilde{\chi(\mathcal{C})}}$ *and* $\mathcal{F}_Y^{\mathcal{D}} \cong \mathcal{F}_Y^{\mathcal{C}} \otimes \mathcal{F}_Y^{\widetilde{\mathcal{C}}}$,

$$\begin{aligned}&\sum_j R_\Phi^{\mathcal{D}}(\psi_Y^{\mathcal{C}} \otimes j \otimes \psi_X^{\chi(\mathcal{C})} \otimes \psi_X^{\widetilde{\chi(\mathcal{C})}}; \phi_Y^{\mathcal{C}} \otimes j \otimes \phi_X^{\chi(\mathcal{C})} \otimes \phi_X^{\widetilde{\chi(\mathcal{C})}})\\ &= R_\Phi^{\mathcal{C}}(\psi_Y^{\mathcal{C}} \otimes \psi_X^{\chi(\mathcal{C})}; \phi_Y^{\mathcal{C}} \otimes \phi_X^{\chi(\mathcal{C})}) \left\langle \psi_X^{\widetilde{\chi(\mathcal{C})}} \middle| \phi_X^{\widetilde{\chi(\mathcal{C})}} \right\rangle\end{aligned} \tag{2.20}$$

A causal box can be equivalently described by the Choi-Jamiołkowski representation of the maps $\Phi^{\mathcal{C}}$ and any set of positive semi-definite sesquilinear forms satisfying Equation (2.20) is a valid causal box. See [18] for a proof of this statement.

2.4.2 Stinespring representation

Stinespring dilation theorem: For every CPTP map $\Phi : \mathcal{L}(\mathcal{H}_A) \to \mathcal{L}(\mathcal{H}_B)$ between finite-dimensional Hilbert spaces $\mathcal{H}_A$ and $\mathcal{H}_B$, there exists an isometry $U_\Phi : \mathcal{H}_A \to \mathcal{H}_{BR} \in Hom(\mathcal{H}_A, \mathcal{H}_B \otimes \mathcal{H}_R)$ for some Hilbert space $\mathcal{H}_R$ such that $\Phi(\rho_A) = tr_R(U_\Phi \rho_A U_\Phi^\dagger)$ holds for all $\rho_A \in \mathcal{H}_A$. U_Φ is called the Stinespring representation of the map Φ. Minimal Stinespring representations are unique up to a unitary transformation. For further details, see [39].

The Stinespring representation generalises also to the infinite dimensional case which leads to the characterisation of the Stinespring representation of a causal box as follows.

Stinespring representation of a causal box ([18], 2017 IEEE): A causal box, $\Phi = \{\Phi^{\mathcal{C}} : \mathfrak{T}(\mathcal{F}_X^{\chi(\mathcal{C})}) \to \mathfrak{T}(\mathcal{F}_Y^{\mathcal{C}})\}_{\mathcal{C} \in \overline{\mathfrak{C}}(\mathcal{T})}$ satisfying Definition 2.3.1 can be equivalently represented by the set of minimal Stinespring representations $\{U_\Phi\}$ satisfying the following condition.

For any $\mathcal{C}, \mathcal{D} \in \overline{\mathfrak{C}}(\mathcal{T})$ *with* $\mathcal{C} \subseteq \mathcal{D}$ *and the minimal Stinespring representations* $U_\Phi^{\mathcal{D}} : \mathcal{F}_X^{\chi(\mathcal{D})} \to \mathcal{F}_Y^{\mathcal{D}} \otimes \mathcal{H}_R$ *and* $U_\Phi^{\mathcal{C}} : \mathcal{F}_X^{\chi(\mathcal{C})} \to \mathcal{F}_Y^{\mathcal{C}} \otimes \mathcal{H}_Q$ *of* $\Phi^{\mathcal{D}}$ *and* $\Phi^{\mathcal{C}}$ *respectively, there exists an isometry* $V : \mathcal{H}_Q \otimes \mathcal{F}_X^{\widetilde{\chi(\mathcal{C})}} \to \mathcal{F}_Y^{\widetilde{\mathcal{C}}} \otimes \mathcal{H}_R$ *such that,*

$$U_\Phi^{\mathcal{D}} = \left(I_Y^{\mathcal{C}} \otimes V\right)\left(U_\Phi^{\mathcal{C}} \otimes I_X^{\widetilde{\chi(\mathcal{C})}}\right) \tag{2.21}$$

A causal box can be equivalently described by the minimal Stinespring representations of the maps $\Phi^{\mathcal{C}}$ and any set of such representations satisfying Equation (2.21) is a valid causal box. Again, we refer the reader to [18] for a formal proof of this statement. A circuit diagram illustrating this as given in [18] is reproduced here in Figure 2.5.

2.4.3 Sequence representation

By recursively decomposing a causal box Φ using Equation (2.21), Φ can be decomposed into an infinite series of isometries $\{V_1, V_2, ...\}$. It is shown in [18] that for every causal box there exists a special decomposition of this kind (i.e., the *sequence representation*) which has the following property: each isometry V_i in the decomposition acts on inputs to the causal box produced within a certain region in $\mathcal{T}$, and produces corresponding outputs at a later, *disjoint* region in $\mathcal{T}$, while possibly updating the state of an internal memory in the process. This allows us to view the causal box as a sequence of disjoint operations and talk about the behaviour of the causal box within each "slice" of the set $\mathcal{T}$. For example taking the set $\mathcal{T}$ to represent a time parameter, a causal box that runs for 10 minutes can equivalently be described by its behaviour in every minute, or every half a minute, or every second, or every infinitesimal fraction of a minute. It provides a causal explanation/causal unraveling for the process represented by the causal box. That being said, although a sequence representation exists for every causal box, it is not always easy to find one. We now present the formal definition of the sequence representation as given in [18] and the figure

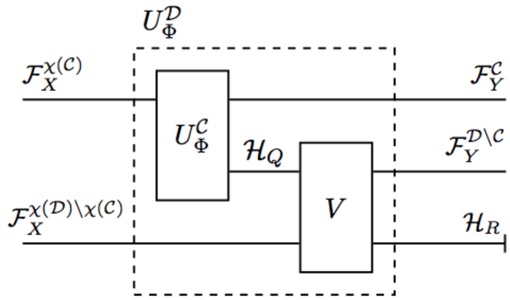


Figure 2.5: **Stinespring representation of a causal box (Figure 8 [18], 2017 IEEE):** "For any $\mathcal{C}, \mathcal{D} \in \overline{\mathfrak{C}}(\mathcal{T})$ with $\mathcal{C} \subseteq \mathcal{D}$, a map $\Phi^{\mathcal{D}} : \mathfrak{T}(\mathcal{F}_X^{\chi(\mathcal{D})}) \to \mathfrak{T}(\mathcal{F}_Y^{\mathcal{D}})$ of a causal box with Stinespring representation $U_\Phi^{\mathcal{D}}$ can be decomposed into a sequence of two isometries $U_\Phi^{\mathcal{C}}$ and V, where $U_\Phi^{\mathcal{C}}$ is a Stinesrping representation of $\Phi^{\mathcal{D}} : \mathfrak{T}(\mathcal{F}_X^{\chi(\mathcal{C})}) \to \mathfrak{T}(\mathcal{F}_Y^{\mathcal{C}})$" [18]

illustrating the sequence representation of a causal box is also taken from [18] and reproduced here as Figure 2.6.

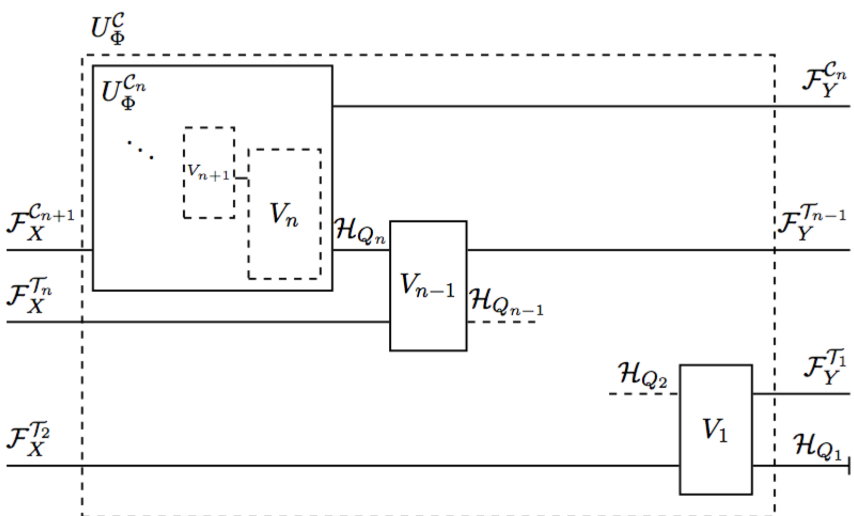


Figure 2.6: **Sequence representation of a causal box (Figure 10 [18], 2017 IEEE):** By repeatedly applying the Stinespring decomposition of Equation (2.21), Figure (2.5), one can decompose a causal box Φ into a finite/infinite sequence of isometries.

Definition 2.4.1 (Sequence representation [18], Definition 5.3, 2017 IEEE). *Let $\mathcal{C}_N \subseteq \ldots \subseteq \mathcal{C}_i \subseteq \ldots \mathcal{C}_1 = \mathcal{C}$ be an finite or infinite ($N = \infty$) sequence of cuts such that $\bigcap_{i=1}^{N} \mathcal{C}_i = \varnothing$,and let $\mathcal{T}_i := \mathcal{C}_i \setminus \mathcal{C}_{i+1}$. A sequence representation of a map $\Phi^{\mathcal{C}} : \mathfrak{T}(\mathcal{F}_X^{\chi(\mathcal{C})}) \to \mathfrak{T}(\mathcal{F}_Y^{\mathcal{C})}$ is given by such a set of cuts $\{\mathcal{C}_i\}_{i=1}^N$ along with a set of operators*

$$\{V_i : \mathcal{H}_{Q_{i+1}} \otimes \mathcal{F}_X^{\mathcal{T}_{i+1}} \to \mathcal{F}_Y^{\mathcal{T}_i} \otimes \mathcal{H}_{Q_i}\}_{i=1}^N,$$

such that for all $n \geq 2$,

$$U_{\Phi}^{\mathcal{C}_1} = \left(\prod_{i=1}^{n-1} I_Y^{\mathcal{C}_{i+1}} \otimes V_i \otimes I_X^{\mathcal{C}_2 \setminus \mathcal{C}_{i+1}} \right) \left(U_{\Phi}^{\mathcal{C}_n} \otimes I_X^{\mathcal{C}_2 \setminus \mathcal{C}_{n+1}} \right), \tag{2.22}$$

where $U_{\Phi}^{\mathcal{C}_i}$ is a minimal Stinespring representation of $\Phi^{\mathcal{C}_i}$.

To ensure that the set of input positions to the operator V_i has an empty intersection with the output positions, we can simply define $\mathcal{C}_i := \chi^{i-1}(\mathcal{C})$ in the sequence representation of any map $\Phi^{\mathcal{C}}$. With this, we will have $\chi(\mathcal{C}_i) \setminus \chi(\mathcal{C}_{i+1}) = \mathcal{T}_{i+1}$ and $\mathcal{T}_{i+1} \cap \mathcal{T}_i = \emptyset$.

2.5 Composition of causal boxes

Causal boxes can be composed by connecting output wires to input wires. To do so, to every causal box Φ one assigns a set of ports, $ports(\Phi)$, through which messages are sent and received. Recall that in the general definition of a causal box (Definition 2.3.1), it was defined with a single input and output wire. This is because one can always use the isomorphism of Equation (2.2) to split a single wire of dimension d into a tensor product of sub-wires whose dimensions sum up to d. For example, a single output wire Y capable of carrying d_Y dimensional systems can be split into two sub-wires, Y_1 and Y_2 capable of carrying d_{Y_1} and d_{Y_2} dimensional systems (with $d_Y = d_{Y_1} + d_{Y_2}$), which can in turn be connected to different causal boxes Ψ and Γ. Arbitrary composition of causal boxes can be achieved by combining the two steps:

1. **Parallel composition:** Two causal boxes Φ and Ψ can be composed in parallel to obtain a new causal box $\Gamma = \Phi \parallel \Psi$ whose input ports are given by the union of the input ports of Φ and Ψ and the output ports are given by the union of the output ports of Φ and Ψ.

2. **Loops:** Selected output ports of the causal box Γ can be connected with suitable input ports to form loops.

We now review the formal definition of these operations.

Definition 2.5.1 (Parallel composition [18], Definition 6.1, 2017 IEEE)**.** *The parallel composition of a (d_A, d_C) causal box $\Phi = \{\Phi^{\mathcal{C}}\}_{\mathcal{C} \in \overline{\mathfrak{C}}(\mathcal{T})}$ and a (d_B, d_D) causal box $\Psi = \{\Psi^{\mathcal{C}}\}_{\mathcal{C} \in \overline{\mathfrak{C}}(\mathcal{T})}$ is defined as the $(d_A + d_B, d_c + d_D)$ causal box $\Gamma = \Phi \parallel \Psi := \{\Phi^{\mathcal{C}} \otimes \Psi^{\mathcal{C}}\}_{\mathcal{C} \in \overline{\mathfrak{C}}(\mathcal{T})}$*

Composition of causal boxes can be achieved by looping the output of a causal box back to one of its input. Lets consider a simple classical example to motivate the general definition that also applies to the quantum case. Consider a classical causal box P given by the set of probability distributions $\{P^{\mathcal{C}}_{DC|AB}\}$ shown in Figure 2.7. The causal box has two classical input wires A and B and two classical output wires C and D. The description of the new system, $Q = \{Q^{\mathcal{C}}_{D|A}\}$ resulting from looping the output wire C to the input wire B can be obtained using:

$$Q^{\mathcal{C}}_{D|A}(d|a) = \sum_{c} P^{\mathcal{C}}_{CD|AB}(c, d|a, c) \tag{2.23}$$

One would naturally ask what guarantees that the new set of distributions $\{Q^{\mathcal{C}}_{D|A}\}$ would be valid, normalised probability distributions. It is shown in [18] that the more general definition (Definition 2.5.2) of loops for all causal boxes (classical, quantum and non-signalling) reduces to Equation (2.23) for classical causal boxes and that the new system is a valid causal box (CPTP map in the general case and normalised distribution in the classical case). In other words, the fact that the system P obeys causality ensures that the new system Q obtained by looping P's outputs to its inputs, is described by a valid set of normalised probability distributions. Loops are in general, defined as follows. Note that only wires/sub-sires of the same dimension can be connected in a loop.

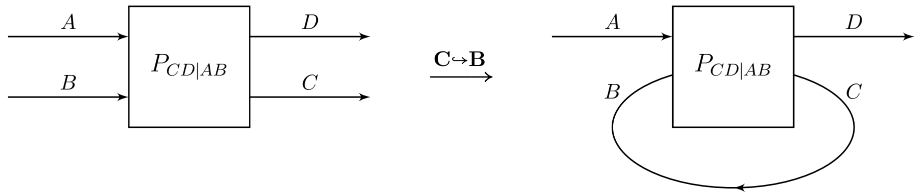


Figure 2.7: **Classical example for loop composition:** A system with classical inputs A, B and classical outputs C, D can be described by the probability distribution $P_{CD|AB}$. The new system obtained by adding a loop from the output C to input B is then described by the distribution $Q_{D|A} = \sum_c P_{CD|AB}(cd|ac)$ and is a valid probability distribution as long as the system obeys causality [18].

Definition 2.5.2 (Loops [18], Definition 6.3, 2017 IEEE)**.** *Let $\Phi = \{\Phi^{\mathcal{C}} : \mathfrak{T}(\mathcal{F}_X^{\chi(\mathcal{C})}) \to \mathfrak{T}(\mathcal{F}_Y^{\mathcal{C}})\}_{\mathcal{C}\in\overline{\mathfrak{C}}(\mathcal{T})}$ be a $(d_A + d_B, d_C + d_D)$-causal box with $d_B = d_C$ and CJ representation $R_\Phi^{\mathcal{C}}(.;.)$. Let $\{|k_C\rangle\}_k$ and $\{|l_C\rangle\}_l$ be any orthonormal bases of $\mathcal{F}_C^{\mathcal{C}}$ and $\{|k_B\rangle\}_k$ and $\{|l_B\rangle\}_l$ denote the corresponding bases of $\mathcal{F}_B^{\mathcal{C}}$, i.e., for all k and l, $|k_C\rangle \cong |k_B\rangle$ and $|l_C\rangle \cong |l_B\rangle$. Putting a loop from the output wire C to the inout wire B results in the new system $\Psi = \Phi^{C\hookrightarrow B}$, is given by the set of maps*

$$\{\Psi^{\mathcal{C}} : \mathfrak{T}(\mathcal{F}_A^{\mathcal{T}}) \to \mathfrak{T}(\mathcal{F}_D^{\mathcal{C}})_{\mathcal{C}\in\overline{\mathfrak{C}}(\mathcal{T})}\}$$

that have the CJ representation

$$R_\Psi^{\mathcal{C}}(\psi_D \otimes \psi_A; \phi_D \otimes \phi_A) = \sum_{k,l} R_\Phi^{\mathcal{C}}(k_C \otimes \psi_D \otimes \psi_A \otimes \bar{k}_B; l_C \otimes \phi_D \otimes \phi_A \otimes \bar{l}_B), \tag{2.24}$$

where $|\bar{k}_B\rangle = \sum_{i=1}^{\infty} |i\rangle \overline{\langle i|k\rangle}$ represents complex conjugation in the basis $\{|i_B\rangle\}_i$ of $\mathcal{F}_B^{\mathcal{T}}$ used in the CJ representation of $\Phi^{\mathcal{C}}$.

These two operations can be combined to define the general composition operation:

Definition 2.5.3 (Composition operation [18], Definition 6.6, 2017 IEEE)**.** *Let Φ and Ψ be two causal boxes with ports(Φ) and ports(Ψ) represent a particular partition of the input and output wires into sub-wires. The set of pairs of ports of Φ and Ψ consisting of an output and input sub-wire of the same dimension with each sub-wire appearing in not more than one pair is denoted by $P = \{(A_1^\Phi, A_1^\Psi), ..., (A_n^\Phi, A_n^\Psi)\}$. Then*

$$\Phi \overset{P}{\longleftrightarrow} \Psi := (\Phi \parallel \Psi)^{(A_1^{\Phi/\Psi} \hookrightarrow A_1^{\Psi/\Phi})\ldots(A_n^{\Phi/\Psi} \hookrightarrow A_n^{\Psi/\Phi})},$$

where $A_i^{\Phi/\Psi} \hookrightarrow A_i^{\Psi/\Phi}$ denotes either $A_i^\Phi \hookrightarrow A_i^\Psi$ or $A_i^\Psi \hookrightarrow A_i^\Phi$ depending on the direction of connection i.e., to which of the two causal boxes the input and output wires correspond to.

Causal boxes are closed under composition i.e., $\Phi \overset{P}{\longleftrightarrow} \Psi$ as defined above is a valid causal box (Proof in [18]).

2.6 Special cases

Definitions 2.2.2 and 2.3.1 define the most general causal box. However, these definitions simplify for certain special cases and we enumerate some of them below.

1. **Totally ordered sets:** When the set $\mathcal{T}$ is totally ordered, the last condition of Definition 2.2.2 to ensure that every point in the set can be reached from any preceding point in a finite number of causal steps namely, $\forall \mathcal{C} \in \overline{\mathfrak{C}}(\mathcal{T}), \forall t \in \mathcal{C}, \exists n \in N\mathbb{N}, t \notin \chi^n(\mathcal{C})$ can be equivalently replaced by the condition:
   For $\chi : \mathcal{T} \to \mathcal{T}$, $inf_{t>t_0}\chi(t) < inf_{t>t_0}t$ and $sup_{t<t_0} < sup_{t<t_0}t$ i.e., the strict inequality $\chi(t) < t$ must also hold in the limit as $t \to t_0$ for every point $t_0 \in \mathcal{T}$.
   (a) **If $\mathcal{T} = \mathbb{Q}$:** the existence of a finite, non-zero delay δ between every input and correlated output is sufficient to satisfy Definition 2.2.2.
   (b) **If $\mathcal{T} \subseteq \mathbb{R}$:** the existence of a $\delta_u > 0$ for every $u \in \mathcal{T}$, such that for all $t \leq u$, $t - \chi(t) > \delta_u$, is equivalent to the fourth condition of Definition 2.2.2.
2. **Finite causal boxes:** In Definition 2.3.1, causal boxes are defined not by a single map but as a set of maps in order to include systems that are well defined within every cut of $\mathcal{T}$ but not on the entire $\mathcal{T}$. Finite causal boxes are the special subset of causal boxes that can be represented by a single map $\Phi : \mathfrak{T}(\mathcal{F}_X^{\mathcal{T}}) \to \mathfrak{T}(\mathcal{F}_Y^{\mathcal{T}})$ that is well defined on the entire set $\mathcal{T}$. In this case the definition of the causality function ensures that all of $\mathcal{T}$ can be reached in a finite number of steps from any $t \in \mathcal{T}$. For this special case, the causality function is defined as follows (taken from Appendix C of [18]):

   Definition 2.6.1 (Finite causality function)**.** *A causality function $\chi : \mathfrak{C}(\mathcal{T}) \to \mathfrak{C}(\mathcal{T})$ is a finite causality function if for every $t \in \mathcal{T}$ there exists an $n \in \mathbb{N}$ such that $t \notin \chi^n(\mathcal{T})$.*

   The trace condition for a finite causal box $\Phi : \mathfrak{T}(\mathcal{F}_X^{\mathcal{T}}) \to \mathfrak{T}(\mathcal{F}_Y^{\mathcal{T}})$ then becomes $tr_{\mathcal{T}\setminus\mathcal{C}} \circ \Phi = \Phi^{\mathcal{C}} \circ tr_{\mathcal{T}\setminus\chi(\mathcal{C})}$.
3. **Minkowski space-time:** When the set $\mathcal{T}$ corresponds to Minkowski space time, all possible cuts are bounded cuts since any two Minkowski space-time points always have a joint causal future that is non-empty.

2.7 Applications

The causal box framework is a general framework for modelling systems that obey causality and are closed under composition. The framework takes a top-down approach where one starts at the highest level of abstraction and introduces only the minimum necessary details/physical specifications at every lower level. For this reason, causal boxes find application in several areas of mathematical physics and information theory as listed in the conclusions section of [18].

For example, causal boxes, being closed under composition naturally lend themselves to modelling composable cryptographic security of relativistic quantum protocols [1]. Cryptographic protocols are said to be composably secure if they remain secure even when used as a subroutine in arbitrary protocols. By combining the causal boxes framework with the abstract cryptography framework [40] and taking set $\mathcal{T}$ to be Minkowski space-time, in [1] we develop a new framework for modelling composable security of relativistic and quantum protocols against quantum and non-signalling adversaries that is also capable of modelling protocols involving superpositions of causal orders. We then prove novel possibility and impossibility results in relativistic quantum cryptography within this framework.

Superpositions of causal orders is a peculiar feature of quantum theory that does not arise classical physics. There are many frameworks for modelling such processes as well as more general processes with indefinite causal order. One such framework namely the process matrix framework [16] models processes that can occur if quantum theory is valid within local laboratories of agents while assuming nothing about the global order of operations performed by different agents. The framework models superpositions such as the quantum switch as well as more general processes that violate so-called causal inequalities [22] which despite being compatible with known physical laws have never been observed in experiments. Causal boxes have a notion of global order hard coded in the framework in the form of the partially ordered set $\mathcal{T}$ and can thus not violate causal inequalities which are derived by dropping the assumption of a fixed global order.

Further, causal boxes could also find interesting applications in the study of quantum complexity and indeterministic systems as explained in [18].

Chapter 3

The process matrix framework [16]

The first ingredient of the process matrix framework is a *local quantum laboratory* within which agents can perform all operations allowed by quantum theory on quantum states that receive from an environment outside the lab, and they can also output a quantum state to the environment. There can be many such local labs within which operations may be ordered according to an agent's local clock but the framework makes no assumptions about any global ordering between the various labs i.e., it is not assumed that these labs are embedded into a fixed space-time structure. The process matrix can then be thought of as a generalised quantum state (density matrix) that models the "outside environment" of the local labs and contains information about how these local labs may be "connected". Causality is then defined in an operational manner without reference to a background space-time: If an agent A is able to influence the measurement outcomes of agent B's operations by preparing suitable quantum states in her local lab, but agent B is never able to influence A's outcomes through any choice of preparation or operation in his local lab, then A is said to causally precede B. We now review the formal definitions of local operations and process matrices and discuss some methods of certifying the non-classicality of causal structures.

3.1 Local quantum laboratory

Each party/agent acts in a *local quantum laboratory* associated with the input Hilbert space $\mathcal{H}_{A_I}$ of dimension d_{A_I} and output Hilbert space $\mathcal{H}_{A_O}$ of dimension d_{A_O}. The dimensions of the input and output spaces need not be the same since the agents could include ancillas prepared in their laboratories or discard certain sub-systems prior to output. However, the Hilbert spaces are assumed to be finite dimensional. The operations performed by agents in their local labs are described by *quantum instruments* [16,21] which are a generalisation of POVMs (positive operator valued measures). Instruments also describe transformations applied to a system in addition to generalised quantum measurements and they reduce to POVMs for 1 dimensional output spaces.

Definition 3.1.1 (Quantum instrument [21])**.** *A quantum instrument $\mathcal{J}^A = \{\mathcal{M}_x^A\}_{x=1}^m$ is a collection of completely positive (CP) maps $\mathcal{M}_x^A : A_I \to A_O$ labelled by the local measurement outcome x, having the property that $\sum_{x=1}^m M_x^A$ is CPTP.*

Here, following the notation of [21], A_I and A_O represent the set of all hermitian, linear operators over $\mathcal{H}_{A_I}$ and $\mathcal{H}_{A_O}$ respectively. In particular, when the classical measurement setting a is used to characterise the operations, the instrument corresponding to each setting is denoted as $\mathcal{J}_a^A = \{\mathcal{M}_{x|a}^A\}_{x=1}^m$.

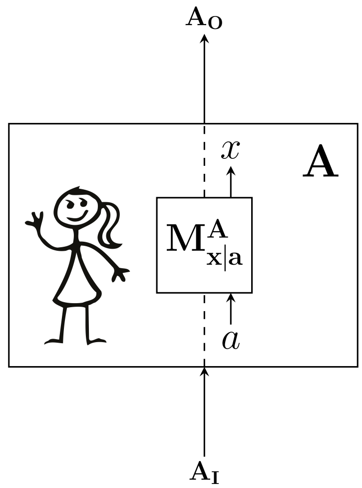


Figure 3.1: **A local quantum laboratory, A:** The local laboratory labelled as A belongs to the experimenter, Alice. The lab can take in an input quantum system belonging to the input space A_I from the outside environment. Alice can then input her local setting choice, a into her device which, depending on this setting performs a CPTP map $M^A_{x|a}$ on the input system, which can have a classical outcome x (as measured on some part of the input system) along with an output quantum system (the part that was not mesured). The output after operation by the CPTP map would be another quantum system belonging to the output space A_O which Alice could then send back into the "outside environment" and she will no longer have control of this system. Now that this local lab has caught your attention, future diagrams of local labs will no longer have a cheerful Alice waving at us; we will also not depict the local settings and outcomes explicitly in diagrams for the sake of simplicity. Henceforth, we will simply represent local labs as boxes with their corresponding name (here, A) along with the input and output arrows corresponding to the spaces A_I and A_O.

Choi Jamiołkowski (CJ) representation of local operations

Every completely positive (CP) map $\mathcal{M} : I \to O$ can be equivalently represented as a positive semi-definite matrix or the CJ matrix in the joint input-output space $I \otimes O$; this is the essence of the CJ isomorphism. In the following sections, we will mostly work in this representation since it is usually easier to work with the CJ representation of a map rather than the map itself. We applied this to causal boxes in Section 2.4 to obtain the CJ representation of a causal box. Likewise, quantum instruments being a set of CP maps also have a corresponding CJ representation. The CJ matrix of a CP map $\mathcal{M}^A_x : A_I \to A_O$ is defined as [21]:

$$M^{A_I A_O}_x := [\mathcal{I} \otimes \mathcal{M}^A_x(|\mathbb{1}\rangle\rangle\langle\langle\mathbb{1}|)]^T \in A_I \otimes A_O \tag{3.1}$$

where $\mathcal{I}$ is the identity map, $|\mathbb{1}\rangle\rangle = |\mathbb{1}\rangle\rangle^{A_I A_I} := \sum_j |j\rangle^{A_I} \otimes |j\rangle^{A_I} \in \mathcal{H}^{A_I} \otimes \mathcal{H}^{A_I}$ is a (non-normalised) maximally entangled state and T denotes partial transpose with respect to the chosen orthonormal basis $\{|j\rangle^{A_I}\}_j$ of $\mathcal{H}^{A_I}$. Note that the the above CJ representation of a quantum instrument has an additional partial transpose as compared to the CJ representation introduced in Section 2.4. This is chosen to obtain a simpler representation of the process matrix (Section 3.2) and does not change the meaning or implication of the representation. A map $\mathcal{M}^A_x$ is completely positive (CP) if its CJ representation is positive semi-definite and is trace preserving (TP) if $tr_{A_O} M^{A_I A_O}_x = \mathbb{1}^{A_I}$ holds (where tr_{A_O} denotes the partial trace over A_O and $\mathbb{1}^{A_I}$ denotes the identity matrix in A_I).

A quantum instrument $\mathcal{J}^A = \{\mathcal{M}_x^A\}_{x=1}^m$ can be equivalently represented by the set $\{M_x^{A_I A_O}\}_{x=1}^m$ satisfying the conditions:

$$M_x^{A_I A_O} \geq 0, \quad tr_{A_O} \sum_{x=1}^{m} M_x^{A_I A_O} = \mathbb{1}^{A_1} \tag{3.2}$$

We now review some properties of the CJ isomorphism as presented in Appendix A1 of [21] which will be useful for the discussion in Chapter 4. In particular, it is useful to differentiate between pure and mixed CJ representations; one provides a representation for linear operators on pure states and the other for maps on density matrices. As we will see, the pure representation takes a more simple form as compared to the general representation, and the former will suffice for describing the quantum switch (Chapter 4).

The pure CJ representation ([21]): For a linear operator $A : \mathcal{H}^{A_I} \to \mathcal{H}^{A_O}$, the CJ representation (or CJ vector in this case) is defined as follows:

$$|A^*\rangle\!\rangle^{A_I A_O} := \mathbb{1} \otimes A^* |\mathbb{1}\rangle\!\rangle, \tag{3.3}$$

where $|\mathbb{1}\rangle\!\rangle \equiv |\mathbb{1}\rangle\!\rangle^{A_I A_I} := \sum_j |j\rangle^{A_1} \otimes |j\rangle^{A_I} \in \mathcal{H}^{A_I} \otimes \mathcal{H}^{A_I}$ (with $\langle\!\langle \mathbb{1}| = |\mathbb{1}\rangle\!\rangle^\dagger$) where $*$ denotes complex conjugation with respect to the chosen orthonormal basis $\{|j\rangle^{A_I}\}_j$ of $\mathcal{H}^{A_I}$. The inverse map is then given by $A|\psi\rangle = [\langle\psi|^{A_I} \otimes \mathbb{1}^{A_O} \cdot |A^*\rangle\!\rangle^{A_I A_O}]^*$. The additional complex conjugation in the definition here (as compared to the usual definition of the CJ representation, Equation (2.15)) is chosen to obtain a simpler representation of the process matrix (Section 3.2).

For example, if the linear operator A is a unitary $U = \sum_{jk} u_{jk} |j\rangle\langle k|$, its CJ vector is given as

$$|U^*\rangle\!\rangle^{A_I A_O} := \mathbb{1} \otimes U^* |\mathbb{1}\rangle\!\rangle = \sum_{jk} u_{jk}^* |k\rangle^{A_I} |j\rangle^{A_O}. \tag{3.4}$$

In this case, U being a unitary is a necessary and sufficient condition for the state $|U^*\rangle\!\rangle^{A_I A_O}$ being maximally entangled [21]. The general case of Equation (3.1) reduces to the particular case of Equation (3.3) for operators of the form $\mathcal{M}^A(\rho) = A\rho A^\dagger$ in which case $M^{A_I A_O} = |A^*\rangle\!\rangle\langle\!\langle A^*|$.
Some examples (Appendix A1 [21])

1. The CPTP map $\mathcal{M}^A(\sigma)$ corresponds to preparing a normalised state ρ at the output irrespective (and independently) of the input state σ and its CJ representation is $M^{A_I A_O} = \mathbb{1}^{A_1} \otimes (\rho^T)^{A_O}$. Note the transpose on ρ.

2. The CP (non-TP) map $\mathcal{M}^A(\rho) = \text{tr}[E\rho]$ that gives the probability of observing a POVM element E in a measurement has an output space of dimension $d_{A_O} = 1$ and is completely described by the CJ representation $M^{A_I} = E^{A_I}$.

3. The CP (non-TP) map $\mathcal{M}^A(\sigma) = \rho\, \text{tr}[E\sigma]$ that represents the map when a POVM element E is measured on the state σ in A_I and a state ρ is prepared in A_O has the CJ representation $M^{A_I A_O} = E^{A_I} \otimes (\rho^T)^{A_O}$.

What we have reviewed so far describes the possible local operations that agents may carry out in their local quantum labs. We will now see how one can calculate joint probabilities involving the settings and outcomes of different agents and what these probabilities can tell us about the nature of interactions between the different agents.

3.2 Process matrices

The probability $P_{X_1,...,X_N|A_1,...,A_N}(x_1,...,x_N|a_1,...,A_N)$ that the N agents A^i observe the outcomes $x_1 \in X_1,...,x_N \in X_N$ for a choice of measurement settings $a_1 \in A_1,...,a_N \in A_N$ respectively is a function of the corresponding CP maps $\mathcal{M}^{A^1}_{x_1|a_1},...,\mathcal{M}^{A^N}_{x_N|a_N}$. As shown in [16, 21], this can be expressed using the CJ representation of the maps as follows

$$\begin{aligned} P_{X_1,...,X_N|A_1,...,A_N}(x_1,...,x_N|a_1,...,A_N) &= P\left(\mathcal{M}^{A^1}_{x_1|a_1},...,\mathcal{M}^{A^N}_{x_N|a_N}\right) \\ &= \mathrm{tr}\left[\left(M^{A^1_I A^1_O}_{x_1|a_1} \otimes ... \otimes M^{A^N_I A^N_O}_{x_N|a_N}\right) W\right] \end{aligned} \tag{3.5}$$

for a hermitian operator $W \in A^1_I \otimes A^1_O \otimes ... \otimes A^N_I \otimes A^N_O$ which is known as the *process matrix*. The set of valid process matrices is characterised by the set of all such hermitian operators that yield positive normalised probabilities for all possible operations including ancillas, tracing out systems and sharing entangled states between multiple agents. It is shown in [21] that this requirement can be expressed in terms of the following conditions that characterise the set of all valid process matrices W. In the following, the notation involving a pre-subscript X with W i.e., ${}_XW$ represents tracing out the sub-system X and replacing it with the normalised identity operator: ${}_XW = \frac{\mathbb{1}^X}{d_X} \otimes \mathrm{tr}_X\, W$.

$$W \geq 0 \tag{3.6a}$$

$$\mathrm{tr}\, W = d_O \tag{3.6b}$$

$$W = L_V(W) \tag{3.6c}$$

where $d_O = d_{A^1_O}...d_{A^N_O}$ and $L_V(W) = {}_{[1-\prod_i(1-A^i_O+A^i_IA^i_O)+\prod_i A^i_IA^i_O]}W$. L_V is a projector onto the linear subspace $\mathcal{L}_V = \{W \in A^1_I \otimes A^1_O \otimes ... \otimes A^N_I \otimes A^N_O | W = L_V(W)$. We now discuss specific examples and particular cases in the following sections which will further clarify this definition.

3.2.1 Pure process matrices [21]

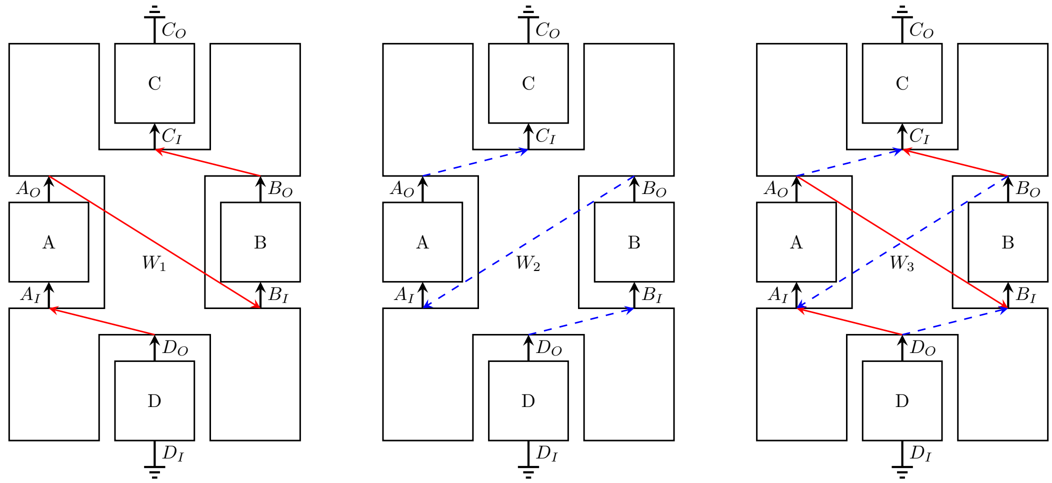
If the process matrix turns out to be a rank-one projector [21], $W = |w\rangle\langle w|$ and the CJ operators representing the local operations are also rank-one projectors (e.g., unitaries and projective measurements followed by pure re-preparations), one can simplify the problem by working at the level of "process vectors" (such as $|w\rangle$) instead of process matrices W and probability amplitudes instead of probabilities. If the local operations of the N labs $A_1,...,A_N$ are represented by the CJ vectors $|A^*_1\rangle\rangle^{A^1_IA^1_O},...,|A^*_N\rangle\rangle^{A^N_IA^N_O}$, the probability given by the general rule, Equation (3.5) reduces to the modulus squared of the following probability amplitude. This is true upto a global phase which can be chosen to be 0.

$$|w\rangle^{A^1_O...A^N_I} = |U_1\rangle\rangle^{A^1_OA^2_I} \otimes ... \otimes |U_N\rangle\rangle^{A^{N-1}_OA^N_I} \tag{3.7}$$

A process matrix for N agents consisting of unitary channels from each agent A_i to the agent A_{i+1} is represented as

$$(\langle\langle A^*_1|^{A^1_IA^1_O} \otimes ... \otimes \langle\langle A^*_N|^{A^N_IA^N_O}) \cdot |w>^{A^1_IA^1_O...A^N_IA^N_O}, \tag{3.8}$$

where $|U_i\rangle\rangle^{A^i_OA^{i+1}_I} = (\mathcal{I} \otimes U)|\mathbb{1}\rangle\rangle$. This represents a pure, causally ordered process matrix with the order $A_1 \prec A_2 \prec ... \prec A_N$.



(a) (b) (c)

Figure 3.2: **Process matrices:** Within the local laboratories A, B, C and D, agents can perform local quantum operations on their corresponding input system and later output another system. No assumption is made about the global ordering of different agents. The process matrix W is an object that contains information about the "outside world", in particular, it contains information about how the different local laboratories are connected (e.g., which lab can signal to which other labs). The process matrix may allow different local labs to be connected in a *superposition of orders*. a) The process matrix W_1 connects the labs in the fixed order $D \prec A \prec B \prec C$ where $A \prec B$ means that A can signal to B. b) The process matrix W_2 connects the labs in the fixed order $D \prec B \prec A \prec C$. c) The process matrix W_3 represents the superposition of the two fixed orders $D \prec A \prec B \prec C$ (solid red arrows) and $D \prec B \prec A \prec C$ (dashed blue arrows) given by the *causally ordered* process matrices W_1 and W_2 respectively and is itself a valid process matrix. In fact, the process matrix of the quantum switch [21] given in Equation (4.7) achieves exactly this. Note that this is in contrast with quantum circuits (e.g., Figure 1.3) where there is always a fixed temporal order of operations.

3.2.2 Non-signalling and signalling process matrices [21]

Here we review the special cases where a process matrix does not allow signalling between any of the agents and where it allows signalling in a fixed direction between agents (for example A can signal to B but B cannot signal to A). When a process matrix W is non-signalling, it does not contain any channels connecting the output space of any of the agents to the input of another and thus acts trivially on all output spaces. In this case, tracing out all the output subsystems should leave the process matrix unchanged [21] and the process matrix is characterised solely by the joint state shared by the different agents i.e., $W = {}_{A_O^1 \cdots A_O^N}W = \rho^{A_I^1 \cdots A_I^N} \otimes \mathbb{1}^{A_O^1 \cdots A_O^N}$. This corresponds the N parties receiving the fixed, joint quantum state $\rho^{A_I^1 \cdots A_I^N}$ from the outside environment and each of them performing their local measurements on their part of the state, without communicating to each other. In this case, the probability rule, Equation (3.5) reduces to the usual Born rule

$$P(M_{x_1|a_1}^{A^1}, \ldots, M_{x_N|a_N}^{A^N}) = \mathrm{tr}\left[\left(E_{x_1|a_1}^{A_I^1}, \ldots, E_{x_N|a_N}^{A_I^N}\right)\rho\right],$$

where $E_{x_i|a_i}^{A_I^i} := \mathrm{tr}_{A_O^i} M_{x_i|a_i}^{A_I^i A_O^i}$ are the POVM elements corresponding to the quantum operation carried out by the different agents.

In the situation where there are N parties $A^1, ..., A^N$, where a party A^i can only signal to a party A^j if $i < j$, the corresponding process matrix W must satisfy the following conditions (derived in [21])

$$\begin{aligned} W &= {}_{A_O^N}W \\ {}_{A_I^N A_O^N}W &= {}_{A_O^{N-1} A_I^N A_O^N}W \\ &. \\ &. \\ &. \\ {}_{A_I^2 A_O^2 \dots A_I^N A_O^N}W &= {}_{A_O^1 A_I^2 A_O^2 \dots A_I^N A_O^N}W. \end{aligned} \tag{3.9}$$

In this case, the process W is compatible with the causal order $A^1 \prec A^2 \prec \dots \prec A^N$ and denotes the *causally ordered* process $W = W^{A^1 \prec A^2 \prec \dots \prec A^N}$. It is shown in [21] that such process (including permutations of the order of parties) can be represented as quantum circuits.

3.2.3 Further examples of process matrices [10]

The following examples are taken from [10]. They illustrate what the process matrices and probability rules look like for certain simple situations.

1. Single laboratory
In the case of a single laboratory A, the most general process matrix is simply $W^{A_I} = \rho^{A_1} \geq 0$. While modelling a single lab, it is enough to consider only a non-trivial input space and a trivial output space: a process matrix describing a single lab must act trivially on its output space since there are no other labs for it to be "connected" to through the outside environment i.e., the process matrix. In this case, CP maps reduce to POVM elements $E^{A_I} \geq 0$ and the generalised Born rule of Equation (3.5) reduces to the usual Born rule: $P(R^{A_I}) = \mathrm{tr}[E\rho]$. This describes the situation where the lab A receives the quantum state ρ from the outside environment, performs a measurement on it and doesn't send anything out into the "environment".

The process matrix describes the "outside environment" of the agents and including the preparation ρ in the description of the process matrix W corresponds to the state being prepared by an environment outside the control of the lab A. One can also consider a situation where an agent prepares his/her choice of state. This can be done by considering an additional lab B with a non trivial output space B_O where an agent can choose to prepare one of the states ρ_i from a set which would correspond to the instruments with the CJ representation $\{(\rho_i^{B_O})^T\}_i$. Lab B can then send the prepared state to lab A where it is measured and the process matrix would simply be $\widetilde{W}^{B_O A_I} = |\mathbb{1}\rangle\!\rangle\langle\!\langle\mathbb{1}|^{B_O A_I}$, if the lab B is connected to the lab A through an identity channel (in general, the process matrix could contain an arbitrary channel.). The generalised Born rule, Equation (3.5) now becomes

$$P(E^{A_I}, (\rho_i^{B_O})^T) = \mathrm{tr}\left[\left(E^{A_I} \otimes (\rho_i^{B_O})^T\right) |\mathbb{1}\rangle\!\rangle\langle\!\langle\mathbb{1}|^{B_O A_I}\right] = \mathrm{tr}[E\rho_i] \tag{3.10}$$

This reduces to the case of the single lab A and fixed, oustide preparation ρ if B prepares $\rho_i = \rho \forall i$. Here, the fact that B influences A is seen by noting that the probability of observing any POVM element $E \neq \mathbb{1}$ in A's lab depends non-trivially on B's instrument $\{(\rho_i^{B_O})^T\}_i$ and the process matrix is compatible with the causal order $B \prec A$.

2. Common cause
Consider two laboratories A and B with non trivial input and output spaces. As per the discussion in Section 3.2.2, a process matrix of the form $W^{AB} = \rho^{A_I B_I} \otimes \mathbb{1}^{A_O B_O}$ describes the situation

where the two labs share the bipartite state ρ^{AB} and are non-signalling. Again the shared state is prepared by an "outside environment" and is fixed. In order to vary the state preparation, we can again consider an additional lab C with trivial input space and non-trivial output space that prepares the bipartite state and the state gets distributed through an identity channel to the labs A and B. Since C can prepare a bipartite state, its output space decomposes as $C_O = C_O^1 \otimes C_O^2$, where the sub-systems C_O^1 and C_O^2 are isomorphic to A_I and B_I respectively. The corresponding process matrix is given by $\widetilde{W}^{ABC} = |\mathbb{1}\rangle\!\rangle\langle\!\langle\mathbb{1}|^{C_O^1 A_I} \otimes |\mathbb{1}\rangle\!\rangle\langle\!\langle\mathbb{1}|^{C_O^2 B_I} \otimes \mathbb{1}^{A_O B_O}$.

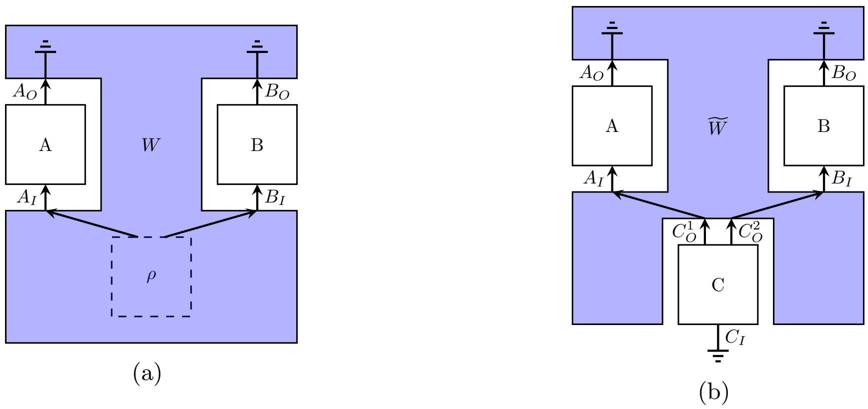


Figure 3.3: **Modelling common cause with process matrices (inspired by Figure 9, [10]):** a) The process matrix $W^{AB} = \rho^{A_I B_I} \otimes \mathbb{1}^{A_O B_O}$ describes two non-signalling laboratories A and B that share a fixed state ρ prepared in their common past. The "earth ground" symbol represents the identity matrix. b) The freedom of preparation choice can be modelled by considering a third lab C that prepares and distributes the states to A and B which is described by the process matrix $\widetilde{W}^{ABC} = |\mathbb{1}\rangle\!\rangle\langle\!\langle\mathbb{1}|^{C_O^1 A_I} \otimes |\mathbb{1}\rangle\!\rangle\langle\!\langle\mathbb{1}|^{C_O^2 B_I} \otimes \mathbb{1}^{A_O B_O}$. This freedom allows C to modify the correlations between A and B by varying his preparation and thus, C is a common cause of A and B.

3. Direct and indirect causes

The previous example of the common cause was that of a bipartite non-signalling process matrix. Here we consider a bipartite, one-way signalling scenario described by the process matrix $W^{AB} = \rho^{A_I} \otimes |U\rangle\!\rangle\langle\!\langle U|^{A_O B_I} \otimes \mathbb{1}^{B_O}$, where U is a unitary matrix and $|U\rangle\!\rangle = \mathcal{I} \otimes U|\mathbb{1}\rangle\!\rangle$. The probability rule of Equation (3.5) now reduces to $tr[(M^{A_I A_O} \otimes N^{B_I B_O})W^{AB}] = tr[FU\mathcal{M}(\rho)U^\dagger]$, where F is obtained by tracing B's output subsystem from the map N implemented in B's lab: $F^{B_I} := tr_{B_O} N^{B_I B_O}$ and $\mathcal{M}$ is the map that the matrix $M^{A_I A_O}$ is the CJ isomorphism (Equation (3.1)) of. This describes a situation where a state ρ is first measured in lab A and after passing through the unitary channel U connecting the labs of A and B, is measured again in B's lab. For arbitrary U and ρ, A can signal to B with appropriate choice of instruments and hence this represents a causally ordered process with the order $A \prec B$.

Again, the connecting mechanism which has a definite order and direction can instead be modelled as an event in a third lab C. For example, if the labs were initially connected by a unitary channel in the bipartite process matrix, this can be seen as a tripartite process matrix where the intervening lab, C performs the corresponding unitary operation. This gives the new process matrix $\widetilde{W}^{ABC} = \rho^{A_I} \otimes |\mathbb{1}\rangle\!\rangle\langle\!\langle\mathbb{1}|^{A_O C_I} \otimes |\mathbb{1}\rangle\!\rangle\langle\!\langle\mathbb{1}|^{C_O B_I} \otimes \mathbb{1}^{B_O}$. The unitary evolution is now represented by the single quantum instrument of C, $|U*\rangle\!\rangle\langle\!\langle U*|^{C_I C_O}$. Note the additional $*$ that appears in the CJ representation when the operation is modelled as an instrument in a local lab, as compared to when it appears as a channel in the process matrix W^{AB}. In this example, the unitary connecting A's output to B's input is not fixed (/hard coded in the process matrix) but can be freely chosen by the intervening lab C. Thus C can break the flow of information from

A to B by using a different instrument[1]; for instance, if C applied the maximally noisy channel $\mathbb{1}^C \backslash d_{C_O}$, then no information from A can travel to B and no choice of instrument of A can affect the probability for any POVM element in B. Thus A is a direct cause of B given the process matrix W^{AB} but is an indirect cause given the process matrix $\widetilde{W}^{ABC}$ [10].

The examples illustrate how process matrices are well-suited for quantum causal modelling [10] as well as for quantum causal discovery algorithms [12]. In classical causal modelling, directed acyclic graphs (DAGs) are widely used to represent the causal structure between a set of random variables (RV) where each node of the graph represents a classical RV and the directed edges represent causal influences. These causal models allow for interventions to be performed on the nodes that change the value of the corresponding RV and also provide a method for calculating the probabilities distribution of other RVs conditioned on the outcome of the intervention on a given set of RVs. As seen in the above examples and the corresponding figures, process matrices allow similar methods to be adapted to the quantum and more general cases. Events in local labs are now taken to represent the nodes of the DAG and the probabilities in the generalised Born rule are easily adapted to define conditional probabilities of interventions [10]. Further, analogous to the trace conditions obtained for signalling and non-signalling process matrices in Section 3.2.2, it is possible to obtain trace conditions for more general causal structures with N agents involving combinations of direct and common cause scenarios. The quantum causal model of [9] which uses the standard quantum formalism (and not the process matrix framework) provides a more general description of the quantum common cause scenario as compared to the quantum causal model of [10] where they provide examples and model quantum common causes whose output space does not factorise into a tensor product, $C_O = C_O^1 \otimes C_O^2$ as shown in Figure 3.3b. Note however that both quantum causal models [10] and [9] can only describe processes with a well-defined causal order and not a superpositions of orders. This is the basis for the first quantum causal discovery algorithm [12]. The algorithm can discover the causal structure of causally ordered as well as probabilistic mixtures of causally ordered processes but there is no known method for causal discovery of "indefinite causal/temporal orders" such as the quantum switch.

Remark. *Note that process matrices do not allow for* causal loops *[16], local or global. No local loops imply that no channel connecting the output and input of the same party can appear in a valid process matrix (for example a term of the kind $|U^*\rangle\!\rangle^{A_O A_I}$ for some unitary U). No global loops imply that terms of the type $|U^*\rangle\!\rangle^{A_O B_I}|V^*\rangle\!\rangle^{B_O A_I}$ which connect A's output to B's input* and *B's output to A's input are forbidden. Note however that the same process matrix can contain these terms in certain kinds of superposition such as the process matrix for the quantum switch, Equation (4.7). A detailed explanation of allowed and forbidden process matrix terms can be found in [16].*

So far we have only considered examples of causally ordered processes. However, process matrices can also contain superpositions of causal orders such as the quantum switch where the causal order of agents is coherently controlled by an additional quantum system. We now discuss the important concepts and tools that allow us to distinguish between causally ordered and unordered processes in a device independent (causal inequalities) or device dependent (causal witnesses) way.

3.3 *Causal* and *non-causal* processes: causal inequalities

Since the process matrix framework allows for classical, quantum and possibly more general processes as well, a natural question to ask is whether one can find certificates of non-classicality (analogous to Bell inequalities [2, 41]) for process matrices solely in terms of the correlations they produce. Causal inequalities [22] do exactly this: they divide the landscape of process matrices into

[1] In a quantum causal model [10], this represents interventions that break the causal arrow from A to B.

two categories, *causal* and *non-causal* processes i.e., those that do not violate a causal inequality and those that do. This is analogous to Bell inequalities that divide hidden variable theories into the categories of *(Bell) local* and *(Bell) non-local* i.e., those that do not violate Bell inequalities and those that do. Note that both causal inequalities as well as Bell inequalities are *device independent* tests of non-classicality: both certify non-classicality of an underlying process solely based on the input-output statistics produced by the process without any assumptions about the underlying theory or devices used.

3.3.1 Bipartite *causal* processes and the (L)GYNI game [22]

Causal correlations [22]
In this section, we will first describe the simplest causal inequality (which can also be expressed as a bound on the winning probability of a bipartite game) as originally presented in the paper [22]. Then we will make the assumptions more explicit by comparing them with the assumptions in the simplest Bell scenario (the bipartite, CHSH game [42]).

Consider an experiment [22] with two parties/agents, Alice and Bob, each of them having control over a local quantum laboratory. Both parties open their lab to let some physical system in, they then interact with it and send a physical system out. This is assumed to happen only once during each run of the experiment. They can choose the classical inputs labeled by a and b and return the classical outputs x and by respectively. All inputs and outputs are assumed to have only a finite number of possible values. The joint conditional probability distribution $p(x,y|a,b)$ describes the input-output correlations established by Alice and Bob through the experiment. Now, if at each run of the experiment, all events of Alice precede all events of Bob, Alice could send her input and output to Bob, but not vice versa. This situation is denoted as $A \prec B$ and there cannot be any signalling from Bob to Alice in this case. The corresponding correlation produced in this case, denoted as $p^{A\prec B}$, must be such that Alice's marginal distribution is independent of Bob's choice of input and we have

$$\forall a,b,b',x, \quad p^{A\prec B}(x|a,b) = p^{A\prec B}(x|a,b'), \tag{3.11}$$

where the marginal is defined as $p^{A\prec B}(x|a,b^{(\prime)}) = \sum_y p^{A\prec B}(x,y|a,b^{(\prime)})$. Similarly, if all events of Bob precede all events of Alice i.e., $B \prec A$, the correlations $p^{B\prec A}$ must satisfy for $p^{B\prec A}(y|a^{(\prime)},b) = \sum_x p^{B\prec A}(x,y|a^{(\prime)},b)$

$$\forall a,a',b,y, \quad p^{B\prec A}(y|a,b) = p^{B\prec A}(y|a',b), \tag{3.12}$$

Note that non-signalling correlations $p(x,y|a,b)$ satisfy both Equations (3.11) and(3.12) and are hence compatible with both $A \prec B$ and $B \prec A$. More generally, we can consider convex mixtures of the above, one-way signalling bipartite distributions to obtain correlations of the form

$$p(x,y|a,b) = qp^{A\prec B}(x,y|a,b) + (1-q)p^{B\prec A}(x,y|a,b) \tag{3.13}$$

for some probability $q \in [0,1]$. According to [21, 22, 43], a bipartite probability distribution $p(x,y|a,b)$ is called "*causal*" if it can be written in the form of Equation (3.13) for some $q \in [0,1]$ and non-negative, normalised distributions $p^{A\prec B}$ and $p^{B\prec A}$ satisfying Equations (3.11) and (3.12) respectively. These are correlations that are obtained when every run of the experiment is compatible with a definite causal order $A \prec B$ or $B \prec A$ which may vary in each run, being determined probabilistically for each run of the experiment. As non-signalling contributions can be included in either $p^{A\prec B}$ or $p^{B\prec A}$, the decomposition Equation (3.13) is in general not unique.

The distributions $p(x,y|a,b)$ satisfying Equation (3.13) correspond to the convex hull (i.e., non-trivial probabilitis mixtures) of the ordered correlations $p^{A\prec B}$ and $p^{B\prec A}$. They form a convex polytope which is known as the *causal polytope* [22]. Just like the *Bell local* polytope [41, 44], the *causal polytope* has certain trivial facets (representing simply the non-negativity or normalisation constraints) as well as non-trivial facets (representing causal inequalities). Analogously, causal inequalities that do not tightly bound causal correlations (3.13) do not correspond to facets of a causal polytope.

A bipartite process matrix $W_{A_I A_O B_I B_O}$ that produces the correlations $p(x, y|a, b)$ (calculated using the probability rule (3.5)) satisfying Equation (3.13) for all choices of instruments $\{M^A_{x|a}\}_{x,a}$ and $\{M^B_{y|b}\}_{y,b}$ of Alice and Bob respectively is called a *bipartite, causal process matrix* [22,43]. Note however that Equation (3.13) does not invoke the underlying process matrix at all, it represents constraints only at the level of the probabilities observed in an experiment. A violation of a causal inequality guarantees in a device independent way that the observed correlation is incompatible with a definite causal order i.e., that it is *non-causal*.

The simplest causal inequality [22]

The minimum number of parties required to talk about a causal order between parties is two. Further, both parties must have non-trivial inputs and outputs i.e., their inputs and outputs must be able to take on at least 2 different values each. If one of the parties had a trivial input or output space, then one of the one-way signalling conditions Equation (3.11) or (3.12) would definitely be satisfied and the distribution would always be compatible with a single definite causal order and hence an extremal point of the causal polytope (see Figure 3.4 for an example). The simplest, non-trivial causal polytope would thus have two parties with inputs and outputs having two different values each (labelled by 0 and 1), analogous to the simplest Bell polytope (the CHSH polytope [42, 44]). In [22] it is shown that this polytope has 112 deterministic vertices and 48 facets of which 16 are trivial (corresponding the the non-negativity constraints $p(x, y|a, b) \geq 0$). The remaining 32 non-trivial facets are divided into two groups of 16 facets each, corresponding to relabelings of the inequalities (3.14) and (3.15) [22]. These constraints represent an upper bound on the winning probability of the *guess your neighbour's input* (GYNI) and *"lazy" guess your neighbor's input* (LGYNI) games achievable by winning strategies that produce correlations satisfying Equation (3.13).

$$\frac{1}{4} \sum_{a,b,x,y} \delta_{x,b} \delta_{y,a} p(x, y|a, b) \leq \frac{1}{2} \tag{3.14}$$

$$\frac{1}{4} \sum_{a,b,x,y} \delta_{a,(x \oplus b)} \delta_{b,(y \oplus a)} p(x, y|a, b) \leq \frac{3}{4} \tag{3.15}$$

where $\oplus$ denotes addition modulo 2.

1. **GYNI:** GYNI is a bipartite game where two parties, Alice and Bob pick uniformly random inputs a and b (i.e., $p(a, b) = \frac{1}{4}$) and they have to output a guess of the other party's input i.e., they win the game if $x = b$ and $y = a$. A bound on the winning probability for this game, for strategies compatible with a definite causal order is obtained in a simple way [22]. If the causal order is $A \prec B$, Bob cannot signal to Alice and Alice cannot know anything about Bob's input bit b and hence $p(x = b) = \frac{1}{2}$ which gives $p(x = b, y = a) \leq \frac{1}{2}$. Similarly for the causal order $B \prec A$, Alice cannot signal to Bob and again, $p(x = b, y = a) \leq \frac{1}{2}$ since $p(y = a) = \frac{1}{2}$. Any convex mixture of these two orders cannot increase the bound on the winning probability and we have

$$p_{GYNI} := p(x = b, y = a) \leq \frac{1}{2}, \tag{3.16}$$

which is the same as Inequality (3.14) for uniform input bits.

2. **LGYNI:** The LGYNI game is the same as GYNI (also with uniform inputs) but for "lazy" Alice and Bob: each party outputs a guess of the other party's input only when their input

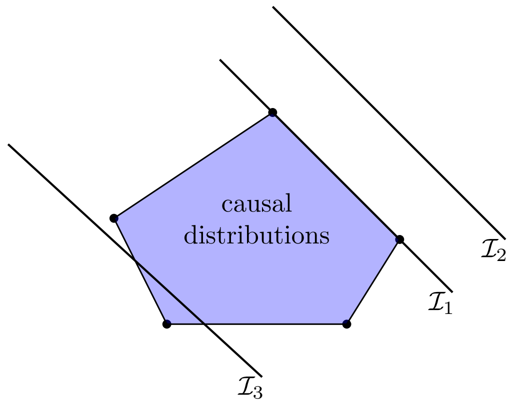


Figure 3.4: **An example of a *causal polytope*:** The causal polytope (blue) is a convex polytope containing the set of all *causal* distributions for a given scenario (fixed number of parties, settings etc.). These are the distributions that are compatible with a fixed causal order (or a classical mixture thereof). A causal inequality is a hyperplane that contains the entire causal polytope on one side: if a distribution is found to be on the side of the hyperplane not containing the causal polytope, it is guaranteed to be "non-classical" in the causal sense i.e., it can't be written as a classical mixture of ordered distributions and is said to be *non-causal* [22, 43]. In this figure, the hyperplane $\mathcal{I}_1$ can correspond to a facet causal inequality since it is one of the facets of the causal polytope while the hyperplane $\mathcal{I}_2$ can also represent a causal inequality, but not a facet causal inequality. On the other hand, the hyperplane $\mathcal{I}_3$ can definitely not be a causal inequality because it does not contain the entire polytope on one side and thus its violation (on either side) would not certify non-classicality of the underlying distribution. The causal polytope can be represented in the vertex representation i.e., as the convex hull of its vertices (deterministic distributions, in this case, 5 of them) or in the facet representation i.e., as the set of distributions satisfying the non-negativity and normalisation constraints and not violating any of the corresponding facet causal inequalities (in this case, a total of 5 constraints, inclusive of non-negativity and normalisation). Note that not all facets of a causal polytope correspond to a facet causal inequality, some correspond to the non-negativity and normalisation constraints that need to be obeyed by all valid probability distributions.

is 1 and outputs an arbitrary bit when their input is 0. The winning probability is bounded in this case as follows and can be obtained with similar reasoning as in the GYNI case.

$$p_{LGYNI} \coloneqq p(a, x \oplus b = 0, b, y \oplus a = 0) \leq \frac{3}{4} \tag{3.17}$$

which is the same as Inequality (3.15) for uniform input bits.

Violation of causal inequalities in the process matrix framework

The inequalities (3.16) and (3.17) are formulated in a theory/framework independent manner. In [22], it is shown that they are violated within the process matrix framework. It was found that for two dimensional input and output systems i.e., $d_{A_I} = d_{A_O} = d_{B_I} = d_{B_O} = 2$, the process matrix

$$W = \frac{1}{4}[\mathbb{1}^{\otimes 4} + \frac{Z^{A_I} Z^{A_O} Z^{B_I} \mathbb{1}^{B_O} + Z^{A_I} \mathbb{1}^{A_O} X^{B_I} X^{B_O}}{\sqrt{2}}] \tag{3.18}$$

with the operations

$$M_{0|0}^{A_I A_O} = M_{0|0}^{B_I B_O} = 0, \tag{3.19a}$$

$$M_{1|0}^{A_I A_O} = M_{1|0}^{B_I B_O} = 2\left|\Phi^+\right\rangle\left\langle\Phi^+\right|, \tag{3.19b}$$

$$M_{1|0}^{A_I A_O} = M_{1|0}^{B_I B_O} = |0\rangle\langle 0| \otimes |0\rangle\langle 0|, \tag{3.19c}$$

$$M_{1|1}^{A_I A_O} = M_{1|1}^{B_I B_O} = |1\rangle\langle 1| \otimes |0\rangle\langle 0|, \tag{3.19d}$$

with $\{|0\rangle, |1\rangle\}$ denoting the eigenbasis of the Pauli Z and $|\Phi^+\rangle := (|00\rangle + |11\rangle)/\sqrt{2}$ violate the inequalities (3.16) and (3.17) with the correlations [22]

$$\begin{aligned} p_{GYNI} &= \frac{5}{16}\left(1+\frac{1}{\sqrt{2}}\right) \approx 0.5335 > \frac{1}{2}, \\ p_{LGYNI} &= \frac{5}{16}\left(1+\frac{1}{\sqrt{2}}\right) + \frac{1}{4} \approx 0.7835 > \frac{3}{4}. \end{aligned} \tag{3.20}$$

As explained in [22], the strategy corresponding to the instruments given in Equations (3.19a)-(3.19d) for the process matrix of Equation (3.18) is: when their input is 0, Alice and Bob simply transmit their incoming physical system, untouched ($2\left|\Phi^+\right\rangle\left\langle\Phi^+\right|$ being indeed the CJ representation of an identity channel), and output the value 1; when their input is 1, Alice and Bob perform a measurement in the Pauli Z basis, whose result defines their classical output, and send out the fixed state $|0\rangle\langle 0|$. Analogously to the CHSH case, one would be interested in finding the maximal violation of these inequalities by solving a suitable optimisation problem and provide "Tsirelson-like" [45] bounds for the same. The important findings and conclusions of [22] in this regard are listed below.

1. The optimisation problem for optimising the violations of the causal inequalities (3.16) and (3.17) for some input and output Hilbert spaces of a given dimension turns out to be non-convex, contrary to the CHSH case [41, 42, 44].

2. From the numerical results of [22], it is conjectured that the maximal violations of these inequalities achievable with qubit systems is

$$\begin{aligned} p_{GYNI}^{max,d=2} &\approx 0.5694 > \frac{1}{2}, \\ p_{LGYNI}^{max,d=2} &\approx 0.8194 = p_{GYNI}^{max,d=2} + \frac{1}{4} > \frac{3}{4} \end{aligned} \tag{3.21}$$

3. Interestingly, the maximal value of p_{GYNI} was found to increase for higher dimensional systems while the maximal value of p_{LGYNI} followed no such increasing trend despite the striking similarity of the two inequalities.

4. Thus the true value of the "Tsirelson bounds" for these two inequalities still remains an open question.

Discussion: assumptions behind Inequalities (3.16) and (3.17)

We will now make explicit the assumptions behind the inequalities (3.16) and (3.17). It would be useful to first review the assumptions behind the CHSH Bell inequality and draw analogies with these causal inequalities. In the CHSH case [42], one again considers two parties, Alice and Bob with inputs a, b and outputs x, y respectively. The Bell local polytope in this case is characterised by all distributions $p(x, y|a, b)$ that satisfy the *local causality* condition (3.22) [41] for some set of hidden variables Λ.

$$p(x, y|a, b) = \int_{\lambda\in\Lambda} q(\lambda) p(a|x, \lambda) p(b|y, \lambda) \tag{3.22}$$

where the (hidden) variables λ are arbitrary variables taking value in a space Λ and distributed according to the probability density $q(\lambda)$. The CHSH game [42] involves two parties, Alice and Bob with with classical input bits a, b and outputs x, y all $\in \{0,1\}$ who are non-signalling (i.e., both Equations (3.11) and (3.12) are satisfied) and choose uniformly random inputs a, b (i.e., $p(a,b) = 1/4$). The game is won if $x \oplus y = a.b$ (where $\oplus$ represents addition modulo 2). The maximum winning probability for local-causal strategies i.e., those that produce correlation satisfying Equation (3.22) is upper bounded as

$$p_{CHSH} \coloneqq p(x, x \oplus a.b|a,b) \leq \frac{3}{4} \tag{3.23}$$

The above inequality rewritten equivalently in terms of the expectation values of the outcomes (which we will not consider here) is usually known as the CHSH inequality [42]. Any classical strategy obeys the Inequality (3.23) as long as no-signalling is satisfied and the inputs are independently and randomly chosen. Often, the latter assumption is known as the *freedom of choice* assumption. We will not go into further details of these assumptions as this would be a chapter of its own and refer the reader to [41] for further information. It was found that the maximally entangled, Bell state, $|\Phi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$ with appropriately chosen measurements for Alice and Bob [42] maximally violate this inequality with a winning probability of $\approx 83\%$ as compared to the "classical" bound of 75% even when the assumptions are satisfied. This implies that quantum theory is *non-local causal* or *Bell non-local*. Note that if one of the assumptions: non-signalling or freedom of choice is not satisfied in an experimental realisation of such a game, even classical strategies can violate the Inequality (3.23) [46].

Coming back to causal inequalities, one notices the analogy between Equations (3.13) and (3.22) and inequalities (3.16), (3.17) and (3.23). Analogous to the *non-signalling* assumption in the CHSH case, there is the "*at most 1-way signalling*" assumption in the GYNI and LGYNI cases. If both way signalling was allowed, both inequalities (3.16), (3.17) could be maximally violated (with a 100% winning probability) even by causally ordered processes by the following trivial strategy: Alice picks an input bit x and sends it to Bob. At the same time, Bob picks his input bit y and sends it to Alice. Upon receiving Bob's input b, Alice outputs $x = b$ and upon receiving Alice's input a, Bob outputs $y = a$. This corresponds to the causal structure shown in Figure 3.5. Such a strategy is avoided only if it is ensured that in each run of the experiment, either all of Alice's operations (i.e., choosing input x and producing output a) are before all of Bob's operations (i.e., choosing input y and producing output b) or all of Bob's operations are before all of Alice's operations. Further, the *freedom of choice* assumption is also required here, just as in the CHSH case: Alice and Bob must choose their inputs x and y independently of each other and they must be uniformly random. Again, if this is not satisfied, a trivial strategy can saturate the logical bound of inequalities (3.16), (3.17) and (3.23): both parties could (prior to the experiment) agree to always prepare the input $a = 0$ and $b = 0$ and produce outputs $x = 0$ and $y = 0$. To summarise, a bipartite process is called *non-causal* if:

1. the following conditions are both satisfied
   (a) **at most 1-way signalling:** The two labs are perfectly isolated and do not leak any information between the time that the input system is received in the lab and the output system is released out of the lab. This guarantees in every round of the experiment that Alice and Bob can not exchange their local setting choices (i.e., two way signalling) and produce their local outcomes after this exchange has been completed.
   (b) **independent inputs:** The local settings of both parties are assumed to be independent of each other and randomly distributed.
2. *and* the process produced statistics that are not compatible with Equation (3.13).

Thus, the interesting case is only when the GYNI and LGYNI inequalities are violated even when the *at most 1-way signalling* and *independent inputs* assumptions are satisfied. Only in this case are the inequalities a device-independent certificate of non-classicality of causal structures and we can infer that the underlying process is truly *non-causal* [22].

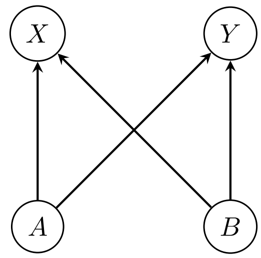


Figure 3.5: The causal ordering of inputs and outputs of Alice and Bob that allow them to trivially violate the GYNI and LGNI causal inequalities. A, B, X and Y ($\in \{0,1\}$) represent the Random Variables of which the corresponding lower case alphabets are specific instances of.

3.3.2 Multipartite scenarios [21]

In a multipartite scenario with N parties $\{A^i\}_{i=1}^N$ with possible setting choices denoted by the vector $\vec{a} = (a_1, ..., a_N)$ and possible outcomes by the vector $\vec{x} = (x_1, ..., x_N)$, multipartite causal inequalities (ref) are constraints on the probability distributions $p(\vec{x}|\vec{a})$ derived from the assumption that there exists an underlying causal structure defining the order between parties. In general, parties appearing earlier in the causal structure can control the order of future parties probabilistically, resulting in a convex combination of correlations compatible with a fixed causal structure. In the case where one party controls the causal order of a set of parties probabilistically [21], *causal* correlations are obtained which decompose into a convex mixture of distributions each compatible with one DAG (i.e., a fixed causal structure) over N nodes (i.e., parties). This general scenario is cumbersome to characterise mathematically for $N > 2$ but takes a much simpler definition (analogous to the bipartite case of Section 3.3.1) for totally ordered causal structures. In the latter case, one obtains *causally ordered* correlations which are special instances of *causal* correlations [21].

Definition 3.3.1 (Causally ordered correlations [21])**.** *Let the set $\mathcal{S} = \{\sigma_i\}_{i=1}^N$ represent the set of all permutations of the N numbers $1, 2, ..., N$. The $N!$ totally ordered DAGs over N nodes correspond to the causal orders $\{A^{\sigma_i(1)} \prec A^{\sigma_i(2)} \prec ... \prec A^{\sigma_i(N)}\}_{i=1}^N$ of the N parties i.e., if the parties act by a permutation $\sigma \in \mathcal{S}$, then the party A^i acts before the party A^j if and only if $\sigma(i) < \sigma(j)$. Then, a probability distribution $p(\vec{x}|\vec{a})$ is compatible with the causal order σ if no party signals to those before her, namely if for every i the marginal distribution*

$$p(x_{\sigma(1)}, ..., x_{\sigma(i)}|\vec{a}) = \sum_{x_{\sigma(j)}, j>i} p(\vec{x}|\vec{a}) \tag{3.24}$$

does not depend on the inputs $a_{\sigma(j)}$ with $j > i$ i.e.,

$$\begin{aligned} &p(x_{\sigma(1)}, ..., x_{\sigma(i)}|a_{\sigma(1)}, ..., a_{\sigma(i)}, a_{\sigma(i+1)}, ..., a_{\sigma(N)}) \\ &= p(x_{\sigma(1)}, ..., x_{\sigma(i)}|a_{\sigma(1)}, ..., a_{\sigma(i)}, a'_{\sigma(i+1)}, ..., a'_{\sigma(N)}) \\ &\qquad \forall a_{\sigma(j)}, a'_{\sigma(j)} \end{aligned} \tag{3.25}$$

A probability distribution that is compatible with at least one causal order σ is said to be causally ordered according to the order σ. More generally, one can have convex combinations of causally *ordered distributions*

$$p(\vec{x}|\vec{a}) = \sum_{\sigma\in\mathcal{S}} q_\sigma p_\sigma(\vec{x}|\vec{a}), \quad q_\sigma \geq 0, \quad \sum_{\sigma\in\mathcal{S}} q_\sigma = 1, \tag{3.26}$$

where each p_σ is compatible with a fixed order $\sigma \in \mathcal{S}$. The set of all correlations $p(\vec{x}|\vec{a})$ satisfying Equation (3.26) are simply referred to as causally ordered correlations.

Note that in the bipartite case (Section 3.3.1), the set of causally ordered and causal correlations coincide since all three possible DAGs over two nodes (Figure 3.6) correspond to total causal orders between the two parties. This is not true when $N > 2$ where there exist many other non-trivial causal structures that are not totally ordered (for example, see Figure 3.7). Note however that Equation (3.26) is a suffiecient (but not necessary) condition for causal separability (Section 3.4) in the multipartite case [21]. We refer the reader to [43, 47] for a more precise characterisation of the causal polytope and corresponding facet inequalities in general multipartite scenarios.

Remark. *There exist process matrices that are "causal" i.e., do not violate a causal inequality but become "non-causal" when they are extended to include some ancilla systems for each party. Hence processes that remain causal even when arbitrary ancillas are included are termed as "extensible causal" [43]. Similarly processes that maintain the property of "causal separability" (Section 3.4) even when ancillas are included are called "extensibly causally separable" [43].*

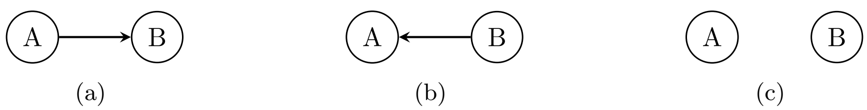


Figure 3.6: **Possible DAGs over two nodes:** a) one way signalling from A to B b) one way signalling from B to A. c) no signalling between A and B.

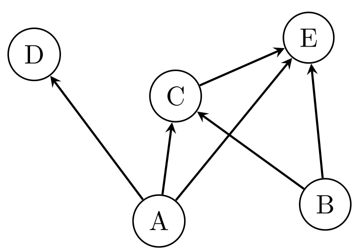


Figure 3.7: **An example of a 5 node DAG.**

3.4 *Causally separable* and *causally non-separable* processes: causal witnesses

In the previous section, we talked about causal orders at the level of probability distributions. Here, we discuss causal orders at the level of process matrices. The former is a *device-independent* approach while the latter is *device-dependent*.

Bipartite causal separability

Definition 3.4.1 (Bipartite causal separability [21]). *A bipartite process matrix $W \in A_I \otimes A_O \otimes B_I \otimes B_O$ is* causally separable *if it can be decomposed as a convex combination of causally ordered processes:*

$$W^{sep} = qW^{A \prec B} + (1-q)W^{B \prec A}, \quad q \in [0,1] \tag{3.27}$$

where $W^{A \prec B}$ and $W^{B \prec A}$ are valid process matrices compatible with the causal orders $A \prec B$ and $B \prec A$ respectively as defined in Section 3.2.2.

Ignoring the normalisation constraint, the set of causally separable process matrices is a convex cone denotes by $\mathcal{W}^{sep}$. A process matrix that cannot be decomposed as in Equation (3.27) is called causally nonseparable.

Special case of tripartite causal separability

The general definition of multipartite causally separable processes with arbitrary dimensions of the output spaces is highly non-trivial, analogous to the case of causal processes (Section 3.3.2). As pointed out in [21], this is because one can consider situations in which an agent, through her local operations, could modify a classical variable that determines the causal order of agents in her future. In such a "classical switch", operations would still be causally ordered in each run of an experiment, but it wouldn't be possible to write the corresponding process matrix as a mixture of valid causally ordered process matrices. A detailed analysis and precise definition of multipartite causal separability can be found in [43]. Here, we define (as given in [21]) a special case of tripartite causal separability for three parties A, B and C where one of the parties, say C has a trivial output space. This definition will be useful when we later review the properties of the quantum switch in Section 4.1.2.

Definition 3.4.2 (Tripartite causal separability (special case) [21]). *Consider three parties A, B and C where C has a trivial output space, i.e., $d_{C_O} = 1$. This means that C cannot signal to the other parties, and every process of this kind must be compatible with C being last and only two definite causal orders are relevant in this case: $A \prec B \prec C$ and $B \prec A \prec C$. In such a situation, a tripartite process matrix $W \in A_I \otimes A_O \otimes B_I \otimes B_O \otimes C_I \otimes C_O$ is* causally separable *if it can be decomposed as a convex combination of causally ordered processes:*

$$W^{sep} = qW^{A \prec B \prec C} + (1-q)W^{B \prec A \prec C}, \quad q \in [0,1] \tag{3.28}$$

where $W^{A \prec B \prec C}$ and $W^{B \prec A \prec C}$ are valid process matrices compatible with the causal orders $A \prec B$ and $B \prec A$ respectively as defined in Section 3.2.2.

Again, ignoring the normalisation constraint, this defines a convex cone $\mathcal{W}^{sep}_{3C}$. Note in general that all *causally separable* process are *causal* processes but the converse is not true. One may consider *causal separability* as analogous to *separability of non-entangled quantum states* (ref) and *causal* processes as analogous to *Bell local* states. The former is a subset of the latter: certain types of non-distillable entanglement is non-separable but may still be Bell local [48, 49] i.e., not violate Bell inequalities.

Causal witnesses [21]

Just as in the case of non-separability of entanglement [48, 49], causal non-separability can also be witnessed as shown in (ref). A causal witness is defined as follows.

Definition 3.4.3 (Causal witness [21]). *A hermitian operator S is called a* causal witness *if $tr[SW^{sep}] \geq 0$ for every causally separable process matrix W^{sep}. The bound 0 and the sign of the inequality are arbitrary, these particular choices are for mathematical convenience.*

Since the set of causally separable processes is closed and convex, for every causally non-separable process matrix W^{ns} there exists a causal witness $S_{W^{ns}}$ such that $tr[S_{W^{ns}}W^{ns}] < 0$. A complete characterisation of causal witnesses is presented in [21].

In order to have an experimental proof of causal non-separability, we must be able to "measure" causal witnesses. This is done by first noting that S is a hermitian operator. Let us consider the bipartite case as done in [21]. The hermitian operator $S \in A_I \otimes A_O \otimes B_I \otimes B_O$ can be decomposed as a linear combination of the form

$$S = \sum_{a,b,x,y} \gamma_{a,b,x,y} M_{x|a}^{A_I A_O} \otimes M_{y|b}^{B_I B_O} \tag{3.29}$$

where $\gamma_{a,b,x,y}$ are real coefficients and $M_{x|a}^{A_I A_O}$ and $M_{y|b}^{B_I B_O}$ are positive semidefinite matrices that can always be interpreted as the Choi-Jamiołkowski representation of CP maps (Section 3.1). Note that this decomposition (3.29) is not unique. We have

$$tr[SW] = \sum_{a,b,x,y} \gamma_{a,b,x,y} tr\left[\left(M_{a|x}^{A_I A_O} \otimes M_{b|y}^{B_I B_O}\right) W\right] \tag{3.30}$$

According to the generalised Born rule of Equation (3.5), the terms $tr\left[\left(M_{x|a}^{A_I A_O} \otimes M_{y|b}^{B_I B_O}\right) W\right]$ represent the probabilities $P(M_{x|a}^{A_I A_O}, M_{y|b}^{B_I B_O})$ that the maps $M_{x|a}^{A_I A_O}$ and $M_{y|b}^{B_I B_O}$ are realised. This allows the causal witness (at least in principle[2]) to be implemented experimentally: one can compute the quantity $tr[SW]$ by implementing the maps $M_{x|a}^{A_I A_O}$ and $M_{b|y}^{B_I B_O}$, estimating the corresponding probabilities $P(M_{x|a}^{A_I A_O}, M_{b|y}^{B_I B_O})$ and combining them as in Equation (3.30). We will discuss a particular example of a causal witness in the Section 4.1.2 about the quantum switch.

3.5 Relation to the two-time states formalism [17]

Typically in quantum mechanics, one prepares a system in a fixed initial state, performs certain operations on it or lets it evolve in time and then measures the final state to record the experimental statistics. This is called *pre-selection*. The two-time formalism [14, 31, 32] describes quantum theory from a perspective where both the initial and final states are fixed. Such a situation could be imagined through *post-selection*: where in an experiment, final states not corresponding to the fixed final state may be discarded and the description of the process on the post-selected ensemble resembles a process where both initial and final states are fixed.

As a concrete example [17], one can consider a situation where an initial state $|\psi\rangle$ is prepared in a lab at time t_1. At some time t between the initial time t_1 and a final time t_2, an observable O is measured on the system prepared in the initial state $|\psi\rangle$. Let the state $|\phi\rangle$ be one of the non-degenerate eigenstates of this observable that can occur with a non-zero probability. The experimenter can now consider the experiment successful if she observes the eigenvalue corresponding to the state $|\phi\rangle$ at time t_2, after measuring O, and discard the system if any other eigenvalue is observed. Thus by repeating the same experiment on an ensemble of particles all prepared in the same initial state, $|\psi\rangle$, the experimenter can obtain a sub-ensemble (post-selected ensemble) of systems with the initial state $|\psi\rangle$ and the final state $|\phi\rangle$. One could then consider the statistics of possible intermediate measurements (between times t_1 and t_2) on the ensemble and this would in general be different for the post-selected and the entire ensemble.

When performing such a quantum experiment, the experimenter can never tell at intermediate times whether the result of the experiment would correspond to the desired final state or which

[2] Of course assuming that these CP maps can be implemented even if the causal order of the parties is not well-defined. In principle, the causal witness for a process matrix can be implemented as long as the process matrix itself can be implemented.

pre- and post-selected ensemble she is working with. She can only know this a-posteriori, at time t_2 after the measurement result has been obtained and the post-selection has been done. On the other hand, if nature allowed for *fundamental post-selection* [17] i.e., where initial and final states of the universe are fixed independently and guaranteed to occur through some natural mechanism, then the experimenter could tell which pre- or post-selected ensemble she is in at times $t_1 < t < t_2$ and see the corresponding statistics, even before the final state is obtained. This is in contrast to *experimental post-selection* described before where there is no guarantee about which final state will occur, however the quantum mechanical predictions for the experimentally post-selected sub-ensemble with initial state $|\psi\rangle$ and final state $|\phi\rangle$ are the same as those for the corresponding fundamental post-selected ensemble. Thus any two time state [17] (described by an initial state $|\psi\rangle$ at time t_1 and final state $|\phi\rangle$ at time t_2) can be prepared in a lab through experimental post-selection.

The main finding of [17] is that process matrices can be directly mapped to a class of two-time states [17] which implies that any process matrix (even those that violate causal inequalities) can be prepared in a lab through experimental post-selection or in other words "the world described by process matrices is equivalent to a particular case of a quantum world with fundamental post-selection" [17]. This provides a physical interpretation of process matrices using laboratory quantum mechanics. However the question of whether all process matrices can be implemented in a lab with pre-selection alone (equivalently if fundamental post-selection exists in our world) still remains open.

Chapter 4

Comparing the two frameworks

Having reviewed the causal boxes and process matrix frameworks, we can now give a preliminary comparison that may be useful for identifying the set of processes that can be described in both formalisms. As explained in Section 1.3, this identification would be useful for understanding the properties of physical causal structures and the physical principles governing them. An exact characterisation of such processes in the intersection of the two frameworks is however, beyond the scope of this work. We now consider a specific example, namely that of the quantum switch introduced in Section 1.4, and compare its representation as a causal box against that as a process matrix.

4.1 A specific example: the quantum switch

A quick recap: the quantum switch a system that performs a quantum-controlled superposition of the orders of two unitaries[1]. The action of the switch is summarised in Equation (4.1) below which is the same as Equation (1.1) and has been reproduced here for convenience. This was experimentally demonstrated in [26, 27] and has been shown to have a computational advantage over causally ordered processes [28, 29] which makes it a particularly interesting case.

$$(\alpha |0\rangle + \beta |1\rangle)_C \otimes |\Psi\rangle_T \to \alpha |0\rangle_C \otimes (U_B U_A |\Psi\rangle)_T + \beta |1\rangle_C \otimes (U_A U_B |\Psi\rangle)_T . \tag{4.1}$$

This can be seen as the action of the global unitary $V(U_A, U_B)$ of the initial state $(\alpha |0\rangle + \beta |1\rangle)_C \otimes |\Psi\rangle_T$ [21].

$$V(U_A, U_B) = |0\rangle\langle 0| \otimes U_B U_A + |1\rangle\langle 1| \otimes U_A U_B, \tag{4.2}$$

where the operator before the tensor product $\otimes$ acts on the control and the operator after the tensor product acts on the target system. Let us now look at how this system is described within the causal boxes and process matrix formalisms.

4.1.1 The quantum switch as a causal box [18]

Here we describe the quantum switch as originally done in [18] i.e., in terms of its sequence representation (Section 2.4.3). In Section 4.1.3, we will rewrite this in the CJ representation (Section 2.4.1) while comparing it with the process matrix for the quantum switch.

[1]The notion of superposition of orders can be easily extended from unitary operations to arbitrary CP maps by allowing parties to operate on ancilla systems. This is because any CP map can be purified to a unitary evolution by introducing an ancillary system and a projective measurement on some subsystem of the original system and ancilla.

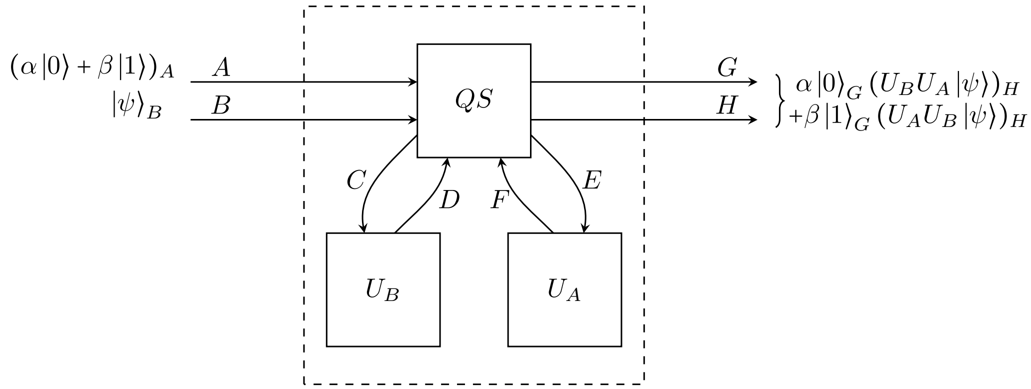


Figure 4.1: **The quantum switch as a causal box (Figure 15 [18])**

As can be seen in Equation (4.1), QS is a system that, given black-box access to two unitaries U_A and U_B, applies them in a controlled superposition of different orders. This is illustrated in Figure 4.1 which is adapted from [18]. Equations (4.1) and (4.2) describe the effect of plugging the quantum switch into the systems U_A and U_B which corresponds to the dashed box from Figure 4.1. However, the quantum switch itself, i.e., the box QS in the figure, cannot be described using combs or circuits while it is a causal box [18].

Firstly, the set $\mathcal{T}$ (here, representing a time parameter) is chosen to be $\mathcal{T} = \{1, 2, ..., 6\}$ since the entire system can be executed in 6 steps. In this case, the causality conditions of Definition (2.2.2) simply require that the output corresponding to an input at t is produced earliest at the next time step, $t+1$. The boxes U_A and U_B can be provided with (internal) counters, that keep track of the number of times that U_A or U_B is applied. Let $|\psi_t^n\rangle \in \vee^n(\mathbb{C}^d \otimes |t\rangle)$ be an element of the symmetric subspace of n qudits all arriving in position t, for $n \geq 1$. Then

$$\begin{aligned} U_A |\Omega\rangle_E \otimes |i\rangle_{U_A} &= |\Omega\rangle_F \otimes |i\rangle_{U_A} \\ U_A |\psi_t^n\rangle_E \otimes |i\rangle_{U_A} &= \left|(U_A^{\otimes n}\psi^n)_{t+1}\right\rangle_F \otimes |i+n\rangle_{U_A} \end{aligned} \tag{4.3}$$

where the register E contains the input to U_A, F contains the output, and the register denoted U_A is the internal counter of the system. The box U_B is defined analogously. A complete description of QS involves knowing how inputs on the entire Fock space of each input wire are mapped to the output space for all points in $\mathcal{T}$. Many of these inputs are "invalid", e.g., the control and target bits are expected to be received at the first step on the wires A and B respectively. Describing the behaviour of QS only on such "valid" inputs suffices, as one can assume that QS simply does nothing if invalid inputs are fed in. The system QS is split into 3 operations at times $t = 1, 3, 5$ [18]:

1. At $t = 1$, QS_1 moves the control qubit to its internal register and forwards the target state $|\psi\rangle$ to either U_A or U_B conditioned on the value of the control.

$$\begin{aligned} QS_1 (|0\rangle_A \otimes |\psi\rangle_B) &= |0\rangle_{QS} \otimes |\Omega\rangle_C \otimes |\psi\rangle_E \\ QS_1 (|1\rangle_A \otimes |\psi\rangle_B) &= |1\rangle_{QS} \otimes |\psi\rangle_C \otimes |\Omega\rangle_E \end{aligned} \tag{4.4}$$

2. At $t = 3$, QS_3 forwards the state received from U_A to U_B and the state received from U_B to U_A.

$$QS_3 (|\psi\rangle_D \otimes |\phi\rangle_F) = |\phi\rangle_C \otimes |\psi\rangle_E \tag{4.5}$$

3. At $t = 5$, QS_5 outputs either the message from U_A or from U_B along with the control qubit,

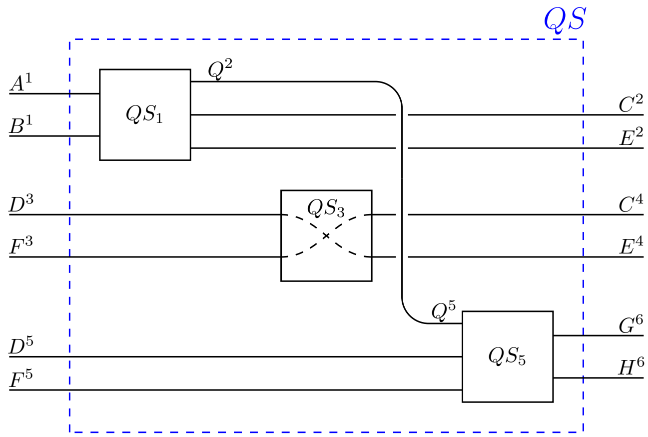


Figure 4.2: **Sequence representation of the quantum switch:** The description of the quantum switch as a causal box provided in this section (which is as given in [18]) is in the sequence representation. Here we illustrate this pictorially. For each wire (including the quantum memory wire Q) $j \in \{A, B, ..., H, Q\}$, $j^t, t \in$ represents the space $\mathbb{C}^2 \otimes \Omega \otimes |t\rangle$ i.e., at most one qubit sent in the corresponding wire at the time t. The wires in the sequence representation are labelled by these spaces. If valid control and target states are sent in wires A^1 and B^1 respectively, QS_1 sends the control on the quantum memory wire Q^2 and the target on E^2 (and $|\Omega\rangle$ on C^2) if the control was $|0\rangle$ and on C^2 (and $|\Omega\rangle$ on E^2) if the control was $|1\rangle$. QS_3 merely connects F^3 to C^4 and D^3 to E^4 as shown. QS_5 takes in the quantum memory Q^5 (unchanged since $t = 2$), connects D^5 to H^6 (discarding F^5) if the memory was $|0\rangle$ and F^5 to H^6 (discarding D^5) if it was $|1\rangle$ and forwards Q^5 to G^6. If the systems U_A and U_B, which implement the corresponding unitaries are plugged between wires E and F and C and D respectively (which act at both $t = 2$ and $t = 4$), one obtains the desired quantum controlled superposition of orders (Section 4.1.1).

conditioned on the value of the control qubit (stored in the internal quantum memory).

$$\begin{aligned} QS_5 \left(|0\rangle_{QS} \otimes |\psi\rangle_D \otimes |\Omega\rangle_F \right) &= |0\rangle_G \otimes |\psi\rangle_H \\ QS_5 \left(|1\rangle_{QS} \otimes |\Omega\rangle_D \otimes |\psi\rangle_F \right) &= |1\rangle_G \otimes |\psi\rangle_H \end{aligned} \tag{4.6}$$

The main Lemma along with proof from [18] which complete the description of the causal box QS are reproduced below.

Lemma 4.1.1 ([18] Lemma 8.1, 2017 IEEE)**.** *The composition of QS, U_A and U_B results in a system which performs a controlled switch between the orders of U_A and U_B where the boxes U_A and U_B are queried only once each.*

Proof. The proof simply consists of putting together all the steps described above. The wires that do not appear in the equations contain a vacuum state in the corresponding step.

$$\begin{aligned}
t = 1 &\qquad (\alpha |0\rangle_A + \beta |1\rangle_A) |\psi\rangle_B |0\rangle_{U_A} |0\rangle_{U_B} \\
t = 2 &\qquad \left(\alpha |0\rangle_{QS} |\Omega\rangle_C |\psi\rangle_E + \beta |1\rangle_{QS} |\psi\rangle_C |\Omega\rangle_E \right) |0\rangle_{U_A} |0\rangle_{U_B} \\
t = 3 &\qquad \alpha |0\rangle_{QS} |\Omega\rangle_D |U_A\psi\rangle_F |1\rangle_{U_A} |0\rangle_{U_B} + \beta |1\rangle_{QS} |U_B\psi\rangle_D |\Omega\rangle_F |0\rangle_{U_A} |1\rangle_{U_B} \\
t = 4 &\qquad \alpha |0\rangle_{QS} |U_A\psi\rangle_C |\Omega\rangle_E |1\rangle_{U_A} |0\rangle_{U_B} + \beta |1\rangle_{QS} |\Omega\rangle_C |U_B\psi\rangle_E |0\rangle_{U_A} |1\rangle_{U_B} \\
t = 5 &\qquad \left(\alpha |0\rangle_{QS} |U_B U_A \psi\rangle_D |\Omega\rangle_F + \beta |1\rangle_{QS} |\Omega\rangle_D |U_A U_B \psi\rangle_F \right) |1\rangle_{U_A} |1\rangle_{U_A} \\
t = 6 &\qquad (\alpha |0\rangle_G |U_B U_A \psi\rangle_H + \beta |1\rangle_G |U_A U_B \psi\rangle_H) |1\rangle_{U_A} |1\rangle_{U_B}
\end{aligned}$$

Thus, in the final step, the wires G and H contain the desired output, and the counters of U_A and U_B are set to 1. □

4.1.2 The quantum switch as a process matrix [23]

In the process matrix framework, the quantum switch can be represented as a four party process matrix [23] between the labs A, B, C and D with the lab C in the global past of all others and lab D in the global future of all others. Here, C prepares the control and target subsystems in her lab and does the following: if the control is in state $|0\rangle$, C sends only the target subsystem to A, who sends it to B after operation, who in turn sends it to D after his operation, and if the control is in state $|1\rangle$, he sends the target to B first, the target goes to B first, then to A and finally to D. C then sends the control subsystem unchanged, directly to D. Note that C lies in the global past of all parties and cannot be signalled to by any of them while D lies in the global future of all parties and cannot signal to any of them; thus C has a trivial input space and D has a trivial output space. Further, C and D send or receive both the control and target qubits, while A and B only receive, operate on and send out the target qubit. The dimensions of input and output systems of the local laboratories are therefore $d_{A_I} = d_{A_O} = d_{B_I} = d_{B_O} = 2, d_{C_I} = 1, d_{C_O} = 4, d_{D_I} = 4, d_{D_O} = 1$. Since C prepares both the control and target qubits (labelled as c and t) and sends them out, its output space can be decomposed as $C_O = C_O^c \otimes C_O^t$ (similar to the decomposition of the output in the common cause example of Section 3.2.3), with $d_{C_O^c} = d_{C_O^t} = 2$. Similarly, since D receives both the control and target qubits (labelled as c and t), its input space can be decomposed as $D_I = D_I^c \otimes D_I^t$, with $d_{D_I^c} = d_{D_I^t} = 2$.

The situation where A receives an arbitrary target state from C_O^t through an identity channel, sends her output to B through an identity channel, who in turn sends his output through an identity channel to D_I^t is represented by the process vector $|\mathbb{1}\rangle\rangle^{C_O^t A_I} |\mathbb{1}\rangle\rangle^{A_O B_I} |\mathbb{1}\rangle\rangle^{B_O D_I^t}$ with $|\mathbb{1}\rangle\rangle = \sum_{j=0} |j\rangle |j\rangle$. Similarly when A and B exchange roles i.e., C sends the target first to B who later forwards it to A and finally to D, we have the process vector $|\mathbb{1}\rangle\rangle^{C_O^t B_I} |\mathbb{1}\rangle\rangle^{B_O A_I} |\mathbb{1}\rangle\rangle^{A_O D_I^t}$. Thus the quantum switch which describes the controlled superposition of the two cases where the first case occurs only when the control (sent directly to D_I^c from C_O^c) is in the $|0\rangle$ state and second only when the control is in the $|1\rangle$ state, is represented by the pure process matrix $W_{QS} = |w_{QS}\rangle \langle w_{QS}|$ where

$$|w_{QS}\rangle = |\mathbb{1}\rangle\rangle^{C_O^t A_I} |\mathbb{1}\rangle\rangle^{A_O B_I} |\mathbb{1}\rangle\rangle^{B_O D_I^t} |00\rangle^{C_O^c D_I^c} + |\mathbb{1}\rangle\rangle^{C_O^t B_I} |\mathbb{1}\rangle\rangle^{B_O A_I} |\mathbb{1}\rangle\rangle^{A_O D_I^t} |11\rangle^{C_O^c D_I^c} \tag{4.7}$$

The situation is illustrated in Figure 4.3. In this case, it can be checked that

$$\begin{aligned} &\left[(\alpha \langle 0| + \beta \langle 1|)^{C_O^c} \otimes \langle \psi^* |^{C_O^t} \otimes \langle\langle U_A^* |^{A_I A_O} \langle\langle U_B^* |^{B_I B_O} \right] |w_{QS}\rangle \\ =&\alpha |0\rangle^{D_I^c} \otimes (U_B U_A |\psi\rangle)^{D_I^t} + \beta |1\rangle^{D_I^c} \otimes (U_A U_B |\psi\rangle)^{D_I^t}, \end{aligned} \tag{4.8}$$

where $\langle \psi^*|$ denotes the complex conjugate of $\langle \psi| = |\psi\rangle^\dagger$ in the computational basis $\{|0\rangle, |1\rangle\}$, such that $\langle \psi^* | i\rangle = \langle i|\psi\rangle, i \in \{0,1\}$. Note that for the control state (in D_O^c), $|\phi\rangle = \alpha |0\rangle + \beta |1\rangle$, $\langle \phi| = |\phi\rangle^\dagger = \alpha^* \langle 0| + \beta^* \langle 1|$ and $\langle \phi^*| = \alpha |0\rangle + \beta |1\rangle$.

Equation (4.8) says that given the process vector $|w_{QS}\rangle$, if C prepares the control and target states as $(\alpha |0\rangle + \beta |1\rangle)$ and $|\psi\rangle$ respectively, while A and B apply the unitaries U_A and U_B respectively, D will end up with the desired final state i.e., the state where the order of the unitaries U_A and U_B acting on the target are entangled with the state of the control. Of course, A and B can choose to apply any other, non-unitary quantum operation/perform measurements on parts of their input system, and the quantum switch would then implement a controlled superposition of these two operations/measurements.

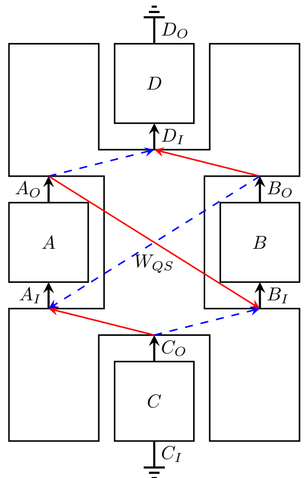


Figure 4.3: **4 party process matrix for the quantum switch:** A lab C in the past of all others (with trivial input space) prepares the control and target states and sends the target to A if the control is in state $|0\rangle$ and to B if the state is $|1\rangle$. After A and B have operated on the target in an order depending on the control state, a lab D in the future of all others (with trivial output space) receives the target from A or B and control directly from D and thereby holds the final state of the joint system where the order of A's and B's operation on the target is entangled with the control state at the end of the process. The process matrix, W for the quantum switch in this case represents a superposition of the orders $C \prec A \prec B \prec D$ (solid red arrows) and $C \prec B \prec A \prec D$ (dashed blue arrows) for the target system.

Note that the reduced process matrix of the quantum switch over A and B only (obtaining by tracing out all of C's and D's inputs and outputs) is just an equal classical mixture of ordered process matrices and is hence causally separable.

$$\begin{aligned} W_{QS}^{AB} &= tr_{C_I C_O D_I D_O} |w_{QS}\rangle \langle w_{QS}| \\ &= \frac{1}{2} W^{A\prec B} + \frac{1}{2} W^{B\prec A}, \end{aligned} \tag{4.9}$$

where

$$\begin{aligned} W^{A\prec B} &= 2(\mathbb{1}^{A_I} \otimes |\mathbb{1}\rangle\!\rangle\langle\!\langle\mathbb{1}|^{A_O B_I} \otimes \mathbb{1}^{B_O}), \\ W^{B\prec A} &= 2(\mathbb{1}^{B_I} \otimes |\mathbb{1}\rangle\!\rangle\langle\!\langle\mathbb{1}|^{B_O A_I} \otimes \mathbb{1}^{A_O}). \end{aligned}$$

Note that all process matrices above are valid process matrices [21] up to normalisation, with the normalisation condition for process matrices being $trW = d_O$, where d_O is the product of the output dimensions of all the labs involved in W.

The causal non-separability of the process matrix (analogous to the non-separability of quantum states) of the quantum switch, W_{QS} is quite evident from Equation (4.7) (since it is a pure, entangled vector) and it can be formally proven by constructing a causal witness S_{QS} (Section 3.4) for W_{QS} and showing that $tr[S_{QS} W_{QS}] \geq 0$. An example of such a witness is the *Chiribella witness* [21]. This witness is based on the result of Chiribella et. al. [50] which shows that quantum controlled superpositions of causal orders such as the QS, provide an operational advantage over classical mixtures of orders in certain information processing tasks. The task considered involves a set of quantum operations such that any two of them either commute or anti-commute and the task itself is to tell whether a given pair of operations commute or anti-commute. This result is remodelled as a causal witness for the quantum switch in [21] by deriving an upper bound on the winning probability for causally separable processes (which include classical mixtures of orders) and showing that the process matrix for the quantum switch exceeds this bound, thereby establishing its causal non-separability.

Inability to violate causal inequalities [21]

Firstly, note that the specific unitaries U_A and U_B are not built in to the description of the quantum switch itself (both in the causal boxes Section 4.1.1 and process matrix Section 4.1.2 frameworks). The quantum switch implements a process that performs a quantum controlled switching between any two operations that one may "plug in" to it (Figures 4.1 and 4.3; these could be unitaries, measurements or other general CPTP maps. When one talks about the quantum switch in the context of causal inequalities (which are formulated in terms of probabilities of measurement outcomes and settings), the local operations performed by each local lab would be a measurement with a corresponding local setting and outcome, but the process matrix used to calculate the corresponding distribution (Equation (3.5)) would be that of the quantum switch (W_{QS}, Equation (4.7)).

We see that the quantum switch clearly does not violate any bipartite causal inequalities such as the GYNI/LGYNI 3.3.1 [22] (Section 3.3.1) for the parties A,B since the reduced process W_{QS}^{AB} (Equation (4.9)) is just a classical mixture of fixed orders and hence causally separable. It can be checked that the reduced process matrix of the quantum switch over any subset of 3 labs is also causally separable by the same argument. Further, it turns out that despite being causally non-separable, W_{QS} does not violate any four party causal inequalities involving A,B, C and D. This is a consequence of the following theorem proved in [21]. We state the theorem here without proof.

Theorem 4.1.1 ([21] Theorem 4)**.** *Consider N+1 parties $\{A^1, ..., A^N, D\}$ with settings $\{a_1, ..., a_N, D\}$ and outcomes $\{x_1, ..., x_N, z\}$. If the marginal distribution $p(\vec{x}|\vec{a}, d) \coloneqq \sum_z p(\vec{x}, z|\vec{a}, d)$ is such that*

1. *$p(\vec{x}|\vec{a}, d) = p(\vec{x}|\vec{a})$ i.e, it does not depend on d: D does not signal to any other (group of) parties;*
2. *$p(\vec{x}|\vec{a}) = \sum_\sigma q_\sigma p_\sigma(\vec{x}|\vec{a})$, where $q_\sigma \geq 0, \sum_\sigma q_\sigma = 1$, and the probability distributions p_σ are causally ordered,*

then the full $(N+1)$-partite probability distribution $p(\vec{x}, z|\vec{a}, d)$ is causal i.e., cannot violate any causal inequalities.

Note that W_{QS} always produces statistics compatible with this theorem for $N = 2$ and $N = 3$: firstly, D does not signal to A or B since $d_{D_O} = 1$, and secondly, any reduced bipartite or tripartite process matrix obtained from W_{QS} is causally separable (an example is given in Equation (4.9)) and can only produce causal correlations that satisfy the second condition of the above theorem. Hence the quantum switch cannot violate any tripartite causal inequalities.

The quantum switch is thus an example of a causally non-separable process that does not violate any causal inequalities i.e., an example of indefinite causal order that can be "witnessed" in a device dependent way but not in a device independent way. This is analogous to the fact that there exist certain entangled states which are non-separable by virtue of being entangled but do not violate Bell inequalities (see [41] and the references therein). All causally non-separable processes known to be physically implementable belong to this category [21]; the interesting question of whether causally non-separable processes that violate causal inequalities can be physically implemented still remains open.

Remark. *Note that the process "vector" for the quantum switch described in [21] is slightly different from the one we describe here (which is also the one used in [23]). In [21], the quantum* *switch is modelled as a tripartite process without a party C in the global past of all others who prepares the control and target states. Instead, the control and target states are hardcoded in the process matrix itself. The four party process vector (Equation (4.7)) used here seems more appropriate because both in the physical implementation and in the causal box description, the control and target can be freely prepared and are not pre-determined by an environment that is outside the experimenter's control. Note that both are equivalent descriptions and that all the results (such as causal non-separability and inability to violate causal inequalities) of [21] also apply to the four party quantum switch considered here [23].*

4.1.3 Comparing the two descriptions of QS

Having reviewed the quantum switch in both frameworks, we can now compare them. Here we show the causal box and process matrix representations of the quantum switch are equivalent up to vacuum states.

The systems U_A and U_B in the causal box description are analogous to the parties A and B in the process matrix description. Further, in order to establish this "equivalence", one needs to rewrite the causal box description of the quantum switch reviewed in Section 4.1.1 in terms of its CJ representation.

The causal box description of the quantum switch [18] (Section 4.1.1) is in terms of the sequence representation for QS which is illustrated in Figure 4.2. Since $\mathcal{T} = \{1, 2, ..., 6\}$, representing time is a totally ordered set, the sets $\mathcal{T}^{\leq t} = \{p \in \mathcal{T} | p \leq t\}$ are equivalent to cuts in this case. The sequence of cuts $\mathcal{C}_N \subseteq ... \subseteq \mathcal{C}_i \subseteq ...\mathcal{C}_1 = \mathcal{C}$ chosen here are $\mathcal{C}_1 = \mathcal{T}^{\leq 6}, \mathcal{C}_2 = \mathcal{T}^{\leq 5}, ..., \mathcal{C}_6 = \mathcal{T}^{\leq 1}$. Hence the sets $\mathcal{T}_i \coloneqq \mathcal{C}_i \backslash \mathcal{C}_{i+1}$ are defined by the single points $\mathcal{T}_i = (7-i), i \in \{1, 2, ..., 6\}$. Further, the causality function is $\chi(t_i) = t_{i-1}$ i.e., $\chi(\mathcal{C}) = \mathcal{C}_{i+1}$. We then have $\mathcal{T}_{i+1} \cap \mathcal{T}_i = \emptyset$, as per the requirement of Definition (2.4.1). Each wire in the sequence representation of Figure 2.6 now carries at most a single message and we can restrict the state space of each wire to the qubit Hilbert space with position information with the vacuum state (no message) included; for each wire $j \in \{A, B, ..., H, \}$, $j^t, t \in$ represents the space $\mathbb{C}^2 \otimes \Omega \otimes |t\rangle$ i.e., qubits sent at the particular time t.

Note that, in the process matrix formalism, each party acts upon a system only once i.e., the target qubit passes through A's and B's lab not more than once each. However, in the casual box description (Figure 4.2), the analogous systems U_A and U_B "act" at two times, ($t = 2$ and $t = 4$). Since one of these operations is on the vacuum state, by definition of QS, both U_A and U_B act on a non-trivial state only once. Since we are dealing with finite dimensional Hilbert spaces, we can simply use the regular CJ representation in terms of the CJ operator instead of the sesquilinear form (Section 2.4.1). From Figure 4.2, QS can be seen as a map $QS_{I\to O}$ from $\mathcal{H}_I \coloneqq A^1 \otimes B^1 \otimes D^3 \otimes F^3 \otimes D^5 \otimes F^5$ to $\mathcal{H}_O \coloneqq C^2 \otimes E^2 \otimes C^4 \otimes E^4 \otimes G^6 \otimes H^6$ and thus its corresponding CJ operator is such that $\Phi_{QS} \in \mathcal{L}(\mathcal{H}_I) \otimes \mathcal{L}(\mathcal{H}_O)$. Further, it turns out that the CJ operator in this case is a rank 1 projector i.e., it can be written as $\Phi_{QS} = |\phi_{QS}\rangle \langle\phi_{QS}|$ for a pure state $|\phi_{QS}\rangle \in \mathcal{H}_\mathcal{I} \otimes \mathcal{H}_\mathcal{O}$. We thus have

$$\begin{aligned} |\phi_{QS}\rangle &= (\mathcal{I}_I \otimes QS_{I\to O}) \sum_{i,...,n\in\{0,1\}} |ijklmn\rangle_I |ijklmn\rangle_I \\ &= \sum_{i,...,n\in\{\Omega,0,1\}} |ijklmn\rangle_I \left(QS_{I\to O} |ijklmn\rangle_I\right), \end{aligned} \tag{4.10}$$

where (Equation (4.10)) we follow the notation $|ijklmn\rangle_I \equiv |i\rangle^{A^1} \otimes |j\rangle^{B^1} \otimes |k\rangle^{D^3} \otimes |l\rangle^{F^3} \otimes |m\rangle^{D^5} \otimes |n\rangle^{F^5}$ and $|ijklmn\rangle_O \equiv |i\rangle^{C^2} \otimes |j\rangle^{E^2} \otimes |k\rangle^{C^4} \otimes |l\rangle^{E^4} \otimes |m\rangle^{G^6} \otimes |n\rangle^{H^6}$. Note that since each set $\mathcal{T}_i$ contains the single element $(7-i), i \in \mathcal{T}$, we can make the notation more compact by not including the time stamp in the state of the system i.e., within the state ket vector, since there is only one possible time at which a message can be sent on each wire in Figure 4.2, which is already given by the label of the wire.

To achieve quantum switching between U_A and U_B, the system U_B should be plugged externally between the wires C and D and U_A between wires E and F, and these connections remain for all times $\mathcal{T}$. Hence the wires labelled C^2 and C^4 in Figure 4.2 are connected to the wires D^3 and D^5 respectively and E^2 and E^4 are connected to F^3 and F^5 respectively. We need not consider cases where the systems U_A or U_B are connected between different combinations of wires since this is not part of the description of the quantum switch presented in Section 4.1.1 [18]. Further, all wires in Figure 4.2 can carry a single qubit or no qubit ($|\Omega\rangle$). However, note that if a vacuum state is sent on the wire A^1, QS will ignore it as this is not a valid input (Section 4.1.1). Hence it is enough to consider the case where a single qubit state is sent on A^1 and we can restrict the basis elements of A^1 to the set $\{0,1\}$ by excluding the vacuum Ω. From Figure 4.2, we have

$$QS_{I\to O} = (QS_1 \otimes \mathcal{I}_{D^3F^3D^5F^5})(QS_3 \otimes \mathcal{I}_{A^1B^1D^5F^5})(QS_5 \otimes \mathcal{I}_{A^1B^1D^3F^3}),$$

Now, wires C and D and wires E and F are at all times, externally connected through some operation and any operation on the vacuum state $|\Omega\rangle$ leaves it unchanged. Noting this, and using Equations (4.4), (4.5) and (4.6), we have

$$\begin{aligned}
|\phi_{QS}\rangle = \sum_{j,\ldots,n\{\Omega,0,1\}} & |0\rangle^{A^1}|j\rangle^{B^1}|k\rangle^{D^3}|l\rangle^{F^3}|m\rangle^{D^5}|n\rangle^{F^5}\left(QS_{I\to O}|0\rangle^{A^1}|j\rangle^{B^1}|k\rangle^{D^3}|l\rangle^{F^3}|m\rangle^{D^5}|n\rangle^{F^5}\right)\\
&+|1\rangle^{A^1}|j\rangle^{B^1}|k\rangle^{D^3}|l\rangle^{F^3}|m\rangle^{D^5}|n\rangle^{F^5}\left(QS_{I\to O}|1\rangle^{A^1}|j\rangle^{B^1}|k\rangle^{D^3}|l\rangle^{F^3}|m\rangle^{D^5}|n\rangle^{F^5}\right)\\
= \sum_{j,\ldots,n\{\Omega,0,1\}} & [\,|0\rangle^{A^1}|j\rangle^{B^1}|k\rangle^{D^3}|l\rangle^{F^3}|m\rangle^{D^5}|\Omega\rangle^{F^5}|\Omega\rangle^{C^2}|j\rangle^{E^2}|l\rangle^{C^4}|k\rangle^{E^4}|0\rangle^{G^6}|m\rangle^{H^6}\\
&+|1\rangle^{A^1}|j\rangle^{B^1}|k\rangle^{D^3}|l\rangle^{F^3}|\Omega\rangle^{D^5}|n\rangle^{F^5}|j\rangle^{C^2}|\Omega\rangle^{E^2}|l\rangle^{C^4}|k\rangle^{E^4}|1\rangle^{G^6}|n\rangle^{H^6}].
\end{aligned} \tag{4.11}$$

Note that in the last step, we have $|\Omega\rangle$ in the wire F^5 whenever we have $|0\rangle$ in the wire A^1. This is because when the control is $|0\rangle$, QS_1 sends $|\Omega\rangle$ to the wire C^2, which remains the unchanged while passing between C^2 and D^3[2] and gets directed into the wire E^4 by QS_3, again remaining unchanged by any operation between E^4 and F^5. Similarly, we also have $|\Omega\rangle$ in the wire D^5 whenever we have $|1\rangle$ in the wire A^1.

Now, following the notation $|\mathbb{1}\rangle\rangle = \sum_j |j\rangle|j\rangle$ used in the process matrix formalism [21] (Section 3.2.1), we have

$$\begin{aligned}
|\phi_{QS}\rangle =& |\mathbb{1}\rangle\rangle^{B^1E^2}|\mathbb{1}\rangle\rangle^{D^3E^4}|\mathbb{1}\rangle\rangle^{F^3C^4}|\mathbb{1}\rangle\rangle^{D^5H^6}|\Omega\Omega\rangle^{C^2F^5}|00\rangle^{A^1G^6}\\
&+|\mathbb{1}\rangle\rangle^{B^1C^2}|\mathbb{1}\rangle\rangle^{F^3C^4}|\mathbb{1}\rangle\rangle^{D^3E^4}|\mathbb{1}\rangle\rangle^{F^5H^6}|\Omega\Omega\rangle^{E^2D^5}|11\rangle^{A^1G^6}.
\end{aligned} \tag{4.12}$$

With the relabelling of systems as in Equation (4.13), one can see that the CJ vector $|\phi_{QS}\rangle$ (Equation (4.12)) of the causal box for QS is identical to the process vector $|w_{QS}\rangle$ (Equation (4.7)) for the quantum switch if the channels that track vacuum states (marked in red in Equation (4.12))

[2] This is because the vacuum state, $|\Omega\rangle$ by definition, remains unchanged under any operation i.e., if "nothing" goes into a system, "nothing comes out!

are ignored.

$$
\begin{aligned}
B^1 &\to C_O^t,\\
E^2, E^4 &\to A_I,\\
F^3, F^5 &\to A_O,\\
C^2, C^4 &\to B_I,\\
D^3, D^5 &\to B_O,\\
H^6 &\to D_I^t,\\
A^1 &\to C_O^c,\\
G^6 &\to D_I^c
\end{aligned}
\tag{4.13}
$$

Now, we define $|U_A^*\rangle\rangle = \mathcal{I} \otimes U_A^* |\mathbb{1}\rangle\rangle$ and $|U_B^*\rangle\rangle = \mathcal{I} \otimes U_B^* |\mathbb{1}\rangle\rangle$ as in the process matrix framework (Section 3.2.1). Since each unitary acts at two distinct times (though only once on a non-vacuum state), we use the notation $|U_A^*\rangle\rangle^{EF} \equiv |U_A^*\rangle\rangle^{E^2F^3} |U^*\rangle\rangle^{E^4F^5}$ and $|U_B^*\rangle\rangle^{CD} \equiv |U_B^*\rangle\rangle^{C^2D^3} |U_B^*\rangle\rangle^{C^4D^5}$. With this, one can easily check that Equation (4.14) holds for $|\phi_{QS}\rangle$, analogous to Equation (4.8) for the process vector $|w_{QS}\rangle$.

$$
\begin{aligned}
&(\alpha \langle 0| + \beta \langle 1|)^{A^1} \otimes \langle \psi^*|^{B^1} \otimes \langle\langle U_A^*|^{EF} \langle\langle U_B^*|^{CD}] \, |\phi_{QS}\rangle \\
=&\alpha \, |0\rangle^{G^6} \otimes (U_B U_A \, |\psi\rangle)^{H^6} + \beta \, |1\rangle^{G^6} \otimes (U_A U_B \, |\psi\rangle)^{H^6},
\end{aligned}
\tag{4.14}
$$

where $\langle \psi^*|$ denotes the complex conjugate of $\langle \psi| = |\psi\rangle^\dagger$ in the computational basis $\{|0\rangle, |1\rangle\}$, such that $\langle \psi^* | i\rangle = \langle i | \psi\rangle, i \in \{0, 1\}$.

The quantum switch is an example involving superpositions of temporal order of operations that can be described using both causal boxes and process matrices. Note that in our analysis of the quantum switch, the sets $\mathcal{T}_i$ in the sequence representation contain single elements. Comparing the sequence representation of a general causal box Φ (Figures 2.6) and that of the quantum switch, QS (Figure 4.2), we see that each wire in the latter case carries a message at a single, fixed time $t \in \{1, ..., 6\}$ and not over a range of times as in the former case. This allowed us to drop the time label and represent a message $|v, t\rangle$ passing through a wire $i^t, i \in \{A, B, C, D, E, F, G, Q\}$ simply as $|v\rangle$ passing through i^t since the time information related to the message is already given in the time label of the wire. Thus, we could simply relabel the wires as in Equation (4.13) and directly map the causal box representation of the quantum switch, $|\phi_{QS}\rangle$ (Equation (4.12)) to its process matrix representation $|w_{QS}\rangle$ (Equation (4.7)) (up to vacuum states). However, a general characterization of processes in the intersection of the two frameworks is still lacking; it is unclear which causal boxes can be mapped to corresponding process matrices (or vice versa) in a similar way, such that they are *mathematically* equivalent. This is because the causal boxes framework explicitly keeps track of the (space-)time stamps in the states which need not always drop out of the state vector as in this special case.

4.1.4 Discussion: mathematical equivalence vs physical interpretation

We have shown that the causal box description (Equation (4.12)) and the process matrix description (Equation (4.7)) of the quantum switch are *mathematically* equivalent up to vacuum states. Note however, that they may be interpreted differently at a *physical* level. The process matrix framework describes the quantum switch as a process where the operations to be superposed are applied within independent isolated labs; performing these operations are modelled as space-time events and it is claimed that corresponding process is an example of *indefinite causal order*. However, in the physical implementation of the quantum switch (Figure 1.3, [26,27]) both unitaries (specific choice of operations) are performed within the same lab and what is achieved is merely a (controlled) *superposition of temporal order* and not a *superposition of causal order*: applying/not applying the first unitary does not *cause* the other unitary to be applied/not applied. Further, the experiments of [26, 27] have a well defined causal explanation in terms of what operations are being performed at each instant of time and they are compatible with a fixed causal ordering of events.

This is better understood in the causal boxes framework, in particular by looking at the sequence representation of the quantum switch (Section 4.1.1, [18]). This representation makes it clear that the physical implementation of the quantum switch implements a *superposition of temporal orders* of operations. This is because it involves the target state passing through each of the boxes U_A and U_B at distinct times: if the control is in state $|0\rangle$, the target passes through U_A at $t = 2$ and U_B at $t = 4$, else it passes through U_B at $t = 2$ and through U_A at $t = 4$ (with vacuum states passing through the other system at each time).

Although the CJ representation of the causal box (Equation (4.12)) appears to be identical to its process matrix representation (Equation (4.7)) through the relabelling of Equation (4.13), the sub-systems in the CJ representation of the causal box are not physically the same as the sub-systems in the corresponding process matrix. In the latter case, the unitaries are assumed to be implemented inside separate, isolated local labs with an inaccessible "outside environment" around them i.e., neither of the labs can control what happens to the target state after the first operation and before the second. These assumptions are not present in the causal box framework where, similar to the physical implementation however, the unitaries can be implemented in the same lab by a single experimenter who can access all three systems QS, U_A and U_B (Figure 4.1) and also freely prepare the control and target states. The process matrix representation appears to have an artificial separation of operations into four parties which doesn't seem to be the case in the physical implementation. However, such a treatment is truly interesting and useful in the case of experiments involving superpositions of gravitating masses [19] where the space-time geometry itself is indefinite. Such experiments have not been realised till date and cannot be modelled in the causal boxes framework and it is definitely a fascinating question to investigate whether they would become possible with future technology.

4.2 A general comparison of the frameworks

In the previous section, we showed that the representation of the quantum switch in the causal box and process matrix framework are mathematically equivalent up to vacuum states for one use of the switch. We also discussed the physical interpretations provided each of the two formalisms for this particular example. In this section, we provide a more detailed and general comparison of the two frameworks which is summarised below in Table 4.1.

	CB [18]	**PM** [16]
Global order	✓	✗
stronger/weaker non-signalling	stronger	stronger
Examples		
Classical, quantum circuits	✓	✓
Quantum switch	✓	✓
PR box	✓	✗
"Non-causal" systems	✗	✓
Applications		
Cryptography	suitable [1]	not suitable
Causal modelling, causal discovery	?	✓(some) [10,12][3]
Superpositions of space-time geometry	✗	✓ [23]
Quantum complexity	?	?

Table 4.1: **A comparison of the causal box (CB) and process matrix (PM) frameworks:** ✓ indicates that an example or application can be modelled within the corresponding framework and ✗ indicates that it can not. ? represents an open question or something that is yet to be tried.

4.2.1 Global and local notions of order, causal inequalities

The process matrix framework only assumes local quantum mechanics (which may be ordered with respect to the time shown by an agent's clock) to be valid in the laboratories of various agents but makes no assumption about any global order between different agents i.e., it does not assume a background "space-time structure". The only condition on process matrices is that they give valid (non-negative and normalised) probabilities for the various operations performed by the agents, which forbids global as well as local causal loops [16]. However, one can have valid process matrices that have no causal description [22] and are not compatible with a fixed background ordering. These are process matrices that violate causal inequalities [22]. In the causal boxes framework on the other hand, although messages can be dynamically ordered, allowing parties to influence the causal order of parties in their future, a global notion of order is still hardcoded in the framework through the partially ordered set $\mathcal{T}$. Thus process matrices have a local notion of order but not a global one while causal boxes have both, the set $\mathcal{T}$ orders all inputs and outputs of a causal box. The existence of a sequence representation for every causal box [18] implies that every causal box can be equivalently described by operations it performs within disjoint subsets

[3]The quantum causal model [10] and the (first) causal discovery algorithm [12] are based on the process matrix framework. Although the framework itself is very general and can model several types of physical and possibly unphysical causal structures, the quantum causal model and causal discovery algorithm presented in these works can only handle definite causal structures. The causal discovery algorithm can not be used even for the physical indefinite causal structures such as the quantum switch. To the best of our knowledge, no known causal model incorporates superpositions of causal orders and no causal discovery algorithm exists for discovering indefinite causal structures.

of $\mathcal{T}$ (e.g., how it behaves within each disjoint time slice) which provides a causal explanation for the underlying process. Note that as discussed in Section 3.3.1, the GYNI and LGYNI causal inequalities can be trivially violated by causal boxes if they are allowed to have space-time stamps compatible with the causal structure of Figure 3.5 i.e., if the parties simply forward their input to the other before the other party produces their output. But one of the implicit assumptions of causal inequalities (discussed in Section 3.3.1) is that in each run of the experiment, either all of Alice's operations must be before all of Bob's or vice versa, in which case causal boxes are not known to violate such inequalities.

4.2.2 Quantum theory applied to gravitating bodies

Indefinite causal structures can arise naturally in thought experiments where one applies the principles of quantum theory to gravitating objects. For example, having a large mass in a superposition of different locations would (according to general relativity) produce a superposition of space-time geometries and consequently, can result in a superposition of causal ordering between events [19].

Such superpositions of the very structure of space-time have been described in [19], where they propose a gravitational implementation of the quantum switch [20] i.e., the *gravitational quantum switch*. The idea behind the gravitational quantum switch is the following:
Consider two local labs A and B (in the absence of a gravitational field) that are initially non-signalling. Now, if a heavy mass, such as a planet is placed close to the local lab A, its gravitational field would cause gravitational time dilation of A's clock which would alter the causal structure between A and B and allow her to signal to B. Likewise, placing the mass instead, next to B would allow B to signal to A. If (hypothetically) the large mass could placed either close to lab A or close to lab B depending coherently on the value of a control quantum state, then one can achieve a controlled superposition of space-time geometry and thereby a controlled superposition of the order of A's and B's operations. This is illustrated in Figure 4.4 which is taken[4] from [19].

Although the gravitational quantum switch appears to be very similar to the quantum switch of Section 4.1.1 [21, 23], there is a major point of difference.

The physical implementation of the quantum switch [26, 27] corresponds to a situation where the target state would enter a local lab (or the particular box performing the unitary) a two distinct times depending on the value of the control: if the control is $|0\rangle$, the target enters lab A at time t_0 and lab B at a strictly later time, t_1 and if the control is $|1\rangle$, the target enters lab B at time t_0 and lab A at the strictly later time, t_1. While at the same time, the vacuum state $|\Omega\rangle$ can be thought of as passing through lab B at t_0 and lab A at t_1 in the first case, and through A at t_0 and B at t_1 in the second case [18].In this case, there is a fixed background space-time structure and the labs and the target state enters each lab at strictly distrinct times depending on the value of the control. Note that such a process has a clear causal explanation i.e., a description of events happening within each interval of time. In fact this is exactly what the sequence representation of the quantum switch (Section 4.1.1) in the causal box framework provides.

In the case of the gravitational switch, however, there is no longer a fixed background space-time structure and local agents measure time with respect to the proper time of their local clocks. In this case, it is shown in [19] that from the perspective of each local agent, the target state enters each lab only at one time t_0 irrespective of the value of the control state and yet, the final state is a controlled superposition of the order of their operations! Such a process can not have a causal explanation from the point of view of the local agents i.e., they can not explain the process happening at each time slice. A distant enough observer, O on whom the gravitational field has negligible effect can describe the events in terms of her co-ordinate time which would be unaffected by the superpositions of the gravitational fields at distant points. O's observations would be compatible with a fixed space-time structure as she would not detect the gravitational

[4]Reproduced here, courtesy of the authors.

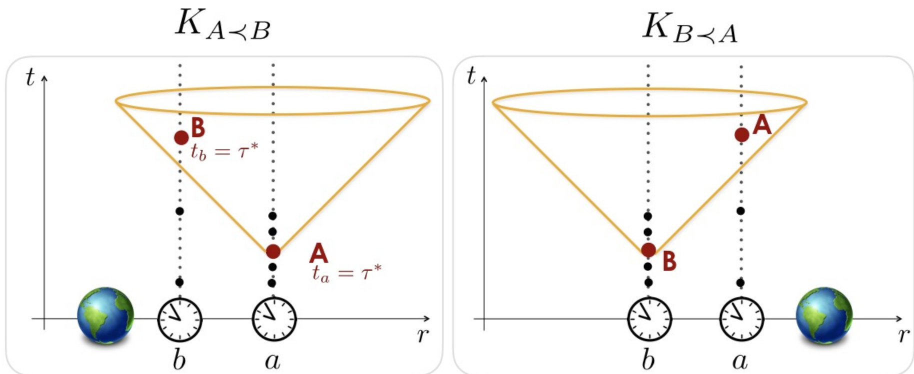


Figure 4.4: **The gravitational quantum switch (Figure 1 [19]):** The gravitational switch is based on the idea that causal relations can be altered by preparing different configurations of a gravitating mass. The clocks a and b are assumed to be initially synchronised and are positioned at fixed distances from a far-away agent O whose time coordinate is t. Events A and B correspond to the clocks at a and b showing the proper time τ. In this figure, the event A corresponds to clock a showing proper time $t_a = \tau = 3units$ and event B corresponds to clock b showing proper time $t_b = \tau = 3units$. Note however that the unit of time measured by each clock would be different due to gravitational time dilation. In the configuration $K^{A \prec B}$, (left) a mass is placed closer to clock b than to a. In this case, gravitational time dilation can cause the event A to end up in the causal past of event B i.e., if long enough proper time has elapsed in each lab, the time difference between the clocks can become larger than the time taken by light to travel between them. The configuration $K^{B \prec A}$ (right) is fully analogous to $K^{A \prec B}$ with the mass placed closer to clock a, in which case the event B ends up in the causal past of the event A.

fluctuations produced at the distant points, and she would observe the target subsystem entering each lab A, B at distinct times and therefore have a causal explanation of the event from her perspective (which would be same as that of the usual quantum switch).

In [19], the example of the gravitational quantum switch is used in a proposal for a *Bell's theorem for temporal order* which is a device-independent but (quantum) theory dependent method for classifying indefinite and definite causal structures. Note that causal inequalities [22] provide a device independent and theory independent way, while causal witnesses [21] provide a device dependent and theory dependent method for doing the same. It is shown [19] that the gravitational quantum switch violates the Bell's theorem for temporal order but not any causal inequality, while the usual quantum switch does not violate causal inequalities [21] or the Bell's theorem for temporal order [19], but it is causally non-separable [21]. Note that one cannot model such superpositions of space-time structure within the causal boxes framework because it assumes a fixed background space-time structure, $\mathcal{T}$ over which all operations are defined.

4.2.3 Quantum and non-signalling processes

Causal boxes can model quantum as well as more general (i.e., "post-quantum") non-signalling systems such as the PR box [51], while process matrices assume that agents perform local quantum operations in their lab, and therefore cannot model a PR box. To be more precise, consider two agents, Alice and Bob with classical inputs a and b and classical outputs x and y respectively and let us take the set $\mathcal{T}$ for the corresponding causal box to be Minkowski space-time. Since the inputs and outputs are classical, the causal box in this case is simply described by the set of classical probability distributions $\{P^{\mathcal{C}}_{XY|AB}\}$. This situation is illustrated in Figure 4.5 in both frameworks.

We now impose space-like separation between the agents so that the no-signalling conditions (i.e., $P_{X|AB}(x|ab) = P_{X|AB}(x|ab')$ for the marginal $P_{X|AB}(x|ab^{(')}) = \sum_y P_{XY|AB}(xy|ab^{(')})$ and similarly for the marginal $P_{Y|AB}(y|a^{(')}b) = \sum_x P_{XY|AB}(xy|a^{(')}b)$) hold. This means that Alice's output cannot depend on Bob's input and vice-versa which imposes a condition on the space-time stamps of the inputs and outputs a, b, x and y of the causal box (Figure 4.6). In such a situation, the PR box correlation $P_{XY|AB}(x, y \oplus a.b|a, b) = 1$ is also a valid causal box, even though it is not known whether a system that produces such correlations between space-like separated parties can ever be physically implemented[5]. However a bipartite process matrix where the parties are non-signalling can only be of the form $W^{AB} = \rho^{A_I B_I} \otimes \mathbb{1}^{A_O B_O}$ or can be written as $\widetilde{W}^{ABC} = |\mathbb{1}\rangle\!\rangle\langle\!\langle\mathbb{1}|^{C_O^1 A_I} \otimes |\mathbb{1}\rangle\!\rangle\langle\!\langle\mathbb{1}|^{C_O^2 B_I} \otimes \mathbb{1}^{A_O B_O}$ by including an additional party in the common past of Alice and Bob who prepares their shared state (see the common cause example of Section 3.2.3). For these process matrices, no operations performed by Alice and Bob in their local labs A and B can violate the Tsirelson's bound [45] and therefore cannot produce the PR box correlations. Note however that if non-signalling is not imposed, these correlations can be trivially generated (even in the process matrix framework) if each party simply forwards their input to the other party before the other party produces their output. Thus, non-signalling process matrices cannot violate corresponding Tsirelson's bounds[6]. This situation for process matrices violating Tsirelson's bounds appears to be analogous to how causal boxes fare with violating causal bounds (i.e., causal inequalities), and it would be interesting to investigate this further to understand how "post-quantumness" in the context of Bell inequalities (i.e., principles governing non-signalling systems that violate Tsirelson's bounds) compares with "post-quantumness" in the context of causal inequalities (i.e., principles governing "non-causal" systems that violate causal inequalities).

4.2.4 Causality vs non-signalling

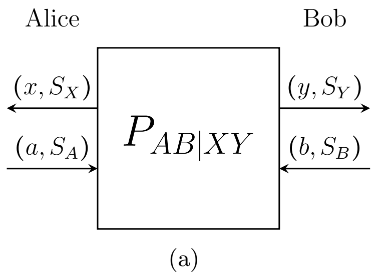
Reference [53] points out that the usual non-signalling constraints (Equation (4.15)) in the multi-party setting are stronger than the constraints arising from relativistic causality alone i.e., the former are sufficient but not necessary conditions for the latter. Starting with a condition for "no causal loops", they argue that only a subset of the stronger non-signalling conditions (4.15) are necessary and sufficient conditions for relativistic causality. Let us call this subset the weak non-signalling constraints. The usual, stronger non-signalling constraints used in multipartite Bell scenarios are given in Equation (4.15) [53]. These are the constrains for an n party scenario with inputs given by the vector $(x_1, ..., x_n)$ and outputs by $(a_1, ..., a_n)$.

$$\begin{aligned}
&\sum_{x_j} P_{X_1,...,X_n|A_1,...,A_n}(x_1, ..., x_j, ..., x_n|a_1, ..., a_j, ..., a_n)\\
=&\sum_{x_j} P_{X_1,...,X_n|A_1,...,A_n}(x_1, ..., x_j, ..., x_n|a_1, ..., a'_j, ..., a_n)\\
&\forall j \in [n], \{x_1, ..., x_n\} \backslash x_j, \{a_1, ..., a_j, a'_j, ..., a_n\}
\end{aligned} \tag{4.15}$$

In words, the above constraints state that the outcome distribution of any subset of parties is independent of the inputs of the complementary set of parties. In the bipartite case (Figure 4.6),

[5]In this scenario, $P_{XY|AB}(x, y \oplus a.b|a, b) \leq \frac{3}{4}$ is a Bell inequality i.e., a system that violates it is certified to be quantum. While the logical bound for this inequality is 1 (which is saturated by the PR box [51]), Tsirelson [45] showed that the quantum bound i.e, the maximum value of $P_{XY|AB}(x, y \oplus a.b|a, b)$ that can be obtained in such a space-like separated experiment (Figures 4.5, 4.6) is close to $0.83 > \frac{3}{4}$. Systems that violate this quantum bound are often called *post-quantum, non-signalling* systems and the PR box is a system that maximally violates this bound. It is not known whether such post-quantum systems are physical.)

[6]Although this is true, it should in principle be possible to extend the process matrix framework to include more general local operations that are compatible with generalised probability theories (GPT e.g., [52]) of which quantum theory is a subset.



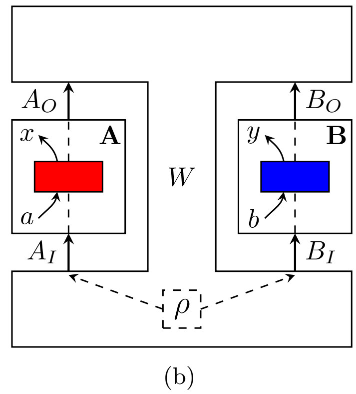


Figure 4.5: **Bipartite process with classical inputs $x \in X$, $y \in Y$ and outputs: $a \in A$,** $b \in B$ (a) as a causal box. S_X, S_Y, S_A and S_B are the corresponding space-time stamps of these messages. (b) as a process matrix. Here Alice can receive a quantum system $\in A_I$ from the outside environment, measure a part of it based on her local setting choice a, produce a corresponding classical output x in her lab and send out a remaining, transformed quantum system $\in A_O$ back into the environment. Similarly, Bob can function identically with his input quantum system $\in B_I$, local setting b, local outcome x and output quantum system $\in B_O$. If Alice's local map (red box) is denoted as $M_{x|a}^{A_I A_O}$ and Bob's local map (blue box) is denoted as $M_{y|b}^{B_I B_O}$, then one can then calculate the corresponding probabilities $P_{XY|AB}(xy|ab)$ using the generalised Born rule (3.5).

these turn out to be necessary and sufficient for relativistic causality i.e., any bipartite correlations generated by space-like separated parties (Figure 4.6) must satisfy Equation (4.15). However, these constraints turn out to be only sufficient for more number of parties i.e., when there are three (or more) space-like separated parties (Figure 4.7), there can exist correlations that do not satisfy Equation (4.15) which still do not contradict relativistic causality. A weaker set of non-signalling conditions which are both necessary and sufficient conditions for relativistic causality are derived in [53].

An example [53] of the weaker condition in the tripartite case would be illustrative to show which one of the strong non-signalling constraints could be dropped in this case without violating relativistic causality between three space-like separated agents. Consider a tripartite Bell scenario with the parties Alice, Bob and Charlie with classical inputs $a \in A$, $b \in B$, $c \in C$ and classical outputs $x \in X$, $y \in Y$, $z \in Z$ respectively, as shown in Figure 4.7. As seen in the Figure, the three parties are space-like separated on a line with Bob in the centre, such that his future light cone contains the intersection of the future light cones of Alice and Charlie. In this setting, the weak non-signalling conditions [53] allow for the joint distribution of outcomes of Alice and Charlie, P_{XZ} to depend on Bob's input, B as long as the marginal distributions P_X of Alice and P_Z of Charlie do not depend on the inputs of complementary sets of parties i.e., P_X does not depend on Bob's or Charlie's inputs B, C and P_Z does not depend on Bob's or Alice's inputs B, A. This means that all dependence on Bob's input must be stored in the correlations between Alice and Charlie and not in their local distributions. These conditions are perfectly compatible with relativistic causality. The intuition behind this is that the joint distribution P_{XZ} and hence the correlations can be accessed by Alice and Charlie only in their joint future which is completely contained in the future of Bob (Figure 4.7). By the time Alice and Charlie can verify the dependence on Bob's input on their joint distribution, they are already in the causal future of Bob's input and there is no superluminal signalling. Thus requiring that the joint distribution of Alice and Charlie also does not depend on Bob's input (as in the strong non-signalling condition) is stronger than what

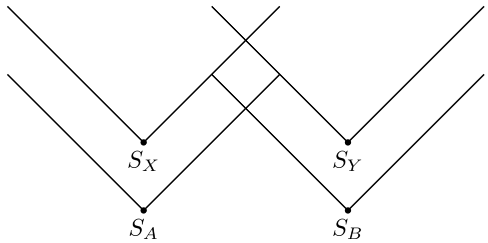


Figure 4.6: **Spacetime diagram for bipartite no-signalling:** Here, time is along the vertical and space along the horizontal and all lines represent light like curves (speed of light, $c = 1$). To impose no-signalling between Alice and Bob, one can space-like separate them as shown here for the bipartite scenario of Figure (4.5). It is important that the spacetime location S_X at which the output X is produced does not lie in the causal future of the location S_B of the input B and similarly that S_Y does not lie in the causal future of S_A.

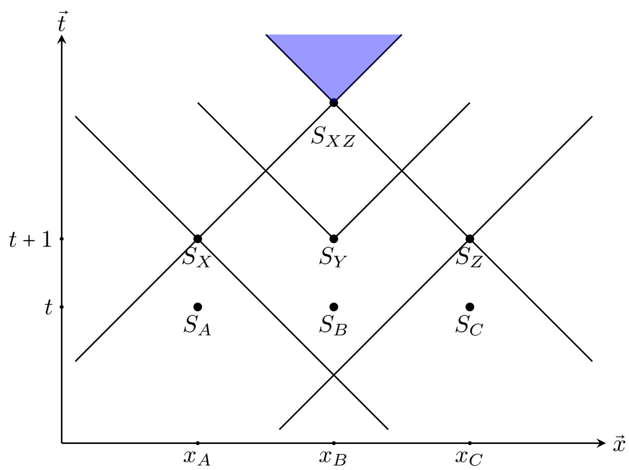


Figure 4.7: **Spacetime diagram for a tripartite Bell scenario:** Three parties Alice, Bob and Charlie are located at the spatial locations x_A, x_B and x_C respectively with Bob in between Alice and Charlie. They generate their inputs A, B, C at time t and produce the corresponding outputs X, Y, Z at time $t+1$, while remaining at their respective spatial locations. $S_i, i \in \{A, B, C, X, Y, Z\}$ denote the space-time points at which the corresponding input/output is generated. Note that the intersection of the future light cones of Alice and Charlie's output points S_X and S_Z (blue region) lies entirely within the causal future of Bob's output point S_Y. Futher, Bob's input point, B does not lie in the causal past of either of Alice's or Charlie's input points, S_A or S_C. In such a scenario, it is shown in [53] that even if the joint distribution of Alice's and Charlie's outcomes, P_{XZ} depends on Bob's input B, relativistic causality can still hold as long as the marginal distributions of individual parties, P_X, P_Y, P_Z do not depend on the inputs of the complementary set of parties. This is because Alice and Charlie can only compute this distribution and verify any B-dependence in the blue region (their joint future), which is entirely in the causal future of B.

relativistic causality demands in this situation. We show here that non-signalling causal boxes impose the stronger no-signalling condition (4.15) working with the example of the same tripartite scenario.

Strong non-signalling in causal boxes

Consider a causal box with the classical inputs $a \in A$,$b \in B$ and $c \in C$, and classical outputs $x \in X$,$y \in Y$ and $z \in Z$ with corresponding space-time stamps (i.e., $\mathcal{T}$ is taken to be Minkowski space) as in Figure 4.7. It is easy to see that such a causal box obeys the stronger non-signalling conditions.

Let $\mathcal{C}$ be the cut upper-bounded by the single point, S_X i.e., $\mathcal{C} = \mathcal{T}^{\leq S_X}$ and the cut $\mathcal{C}$ simply represents the past light cone of the point S_X (including the point itself) in Figure 4.7. Similarly let $\mathcal{D} = \mathcal{T}^{\leq S_Z}$ in which case $\mathcal{D}$ simply represents the past light cone of the point S_Z (including the point itself) in Figure 4.7. Now, by definition of the causality function (Definition 2.2.2), $\chi(\mathcal{C}) \subset \mathcal{C}$, $\chi(\mathcal{D}) \subset \mathcal{D}$ and $\chi(\mathcal{C} \cup \mathcal{D}) = \chi(\mathcal{C}) \cup \chi(\mathcal{D})$. $\chi(\mathcal{C}) \subset \mathcal{C}$ and $\chi(\mathcal{D}) \subset \mathcal{D}$ imply that the outputs X and Z can only depend on inputs produced in their corresponding causal pasts. $\chi(\mathcal{C} \cup \mathcal{D}) = \chi(\mathcal{C}) \cup \chi(\mathcal{D})$ implies that the outputs X and Z together can be described entirely by inputs produced in the union of their causal pasts. Since the input B does not lie in the causal past of either of these points (and therefore not in the union), the joint distribution $P_X Z$ would not depend on B in this case. Thus a tripartite causal box with classical inputs and outputs and corresponding space-time labels as in Figure 4.7 obeys the strong non-signalling conditions, Equation (4.15).

It should be possible to model non-signalling systems compatible with the weaker definition of [53] within the causal boxes framework by weakening the causality conditions. This could be done by dropping the first condition, Condition (2.12a) of Definition 2.2.2 in favour of a weaker condition. In our specific example of Figure 4.7, the weaker condition should model the following fact: the outputs X and Z separately depend only on inputs in their corresponding causal pasts but together, they can depend on inputs in the causal past of the earliest point, S_{XZ} at which the two outputs can be accessed simultaneously (this would be the earliest point in their joint causal future, depicted as the blue region in Figure 4.7). Thus for this particular case, the condition $\chi(\mathcal{C} \cup \mathcal{D}) = \chi(\mathcal{T}^{\leq S_{XZ}})$ could be a substitute for Condition (2.12a) such that the corresponding causal box can model weaker non-signalling systems. Here the point S_{XZ} has the property that $\mathcal{C} \subset \mathcal{T}^{\leq S_{XZ}}$ and $\mathcal{D} \subset \mathcal{T}^{\leq S_{XZ}}$ while $\mathcal{C} \notin \mathcal{T}^{\leq S'}$, $\mathcal{D} \notin \mathcal{T}^{\leq S'}$ or both for any $S' < S_{XZ}$. It would be interesting to see what the weaker causality condition would be in the general case. This could allow causal boxes to model post-quantum cryptographic protocols analysed in [53] where adversaries are restricted by relativistic causality alone.

Strong non-signalling in process matrices

It is easy to see that a tripartite non-signalling process matrix, W_{tri} (see Section 3.2.2 for the definition of non-signalling process matrices) would produce correlations (obtained by plugging it into the probability rule (3.5)) that satisfy the strong non-signalling conditions (4.15). To see this, note that a general tripartite, non-signalling matrix can be written as $W_{tri} = \rho^{A_I B_I C_I} \otimes \mathbb{1}^{A_O B_O C_O}$ (analogous to the bipartite non-signalling process matrix W^{AB} of Section 3.2.3). Thus, for arbitrary local maps with CJ representations (Section 3.1) $M_{x|a}^{A_I A_O}$, $M_{y|b}^{B_I B_O}$ and $M_{z|c}^{C_I C_O}$ (where $a \in A, b \in B$ and $c \in C$ are the particular setting choices and $x \in X, y \in Y$ and $z \in Z$ are the corresponding outcomes observed) that the three parties could perform, the generalised Born rule (3.5) for this case becomes,

$$P_{XYZ|ABC}(xyz|abc) = tr\left[\left(M_{x|a}^{A_I A_O} \otimes M_{y|b}^{B_I B_O} \otimes M_{z|c}^{C_I C_O}\right)\rho^{A_I B_I C_I}\right] \tag{4.16}$$

It can now be readily seen that marginalising the above joint probability distribution to obtain a distribution over the outputs X and Z, by summing over all values y the output Y makes it independent of the input B as well. This is because the b dependence on the right hand side of Equation (4.16) drops out by using $\sum_{y \in Y} M_{y|b}^{B_I B_O} = \mathbb{1}^{B_I}$ (see Equation (3.2)). Thus process matrices also satisfy the stronger non-signalling conditions (4.15). This should not come as a surprise since it was noted in Section 4.2.3 that process matrices in particular cannot model post-quantum, non-signalling systems such as the PR box since the framework assumes local quantum operations. The possibility of modelling PR boxes and more general non-signalling systems [53] in the process matrix framework by replacing local quantum operations with more generalised local operations is yet to be investigated.

4.2.5 Superposition of numbers of messages

The causal box framework models situations where different agents can exchange a superposition of different number of messages in a superposition of orders which may be chosen dynamically during run-time. This is achieved by modelling the state-space of wires as a symmetric Fock space (Chapter 2) and including "space-time stamps" on every message. The process matrix framework does not allow for superpositions of different numbers of messages to be exchanged between agents, since input and output spaces of local laboratories are modelled as Hilbert spaces and not Fock spaces. Thus the framework does not in particular allow for superpositions of sending a state that is a superposition of sending "nothing" and "something" at the same time; such superpositions are important in the physical implementation of controlled unitary operations [35,38] as noted in [18].

4.2.6 Composable relativistic quantum cryptography

Causal boxes are very suitable for modelling several kinds of multi-round cryptographic protocols against a general class of adversaries (classical, quantum and non-signalling) [1]. By virtue of being closed under composition, they can be used to model *composable security* which is a notion of cryptographic security that allows protocols to be securely composed with each other [1,40,54]. In the process matrix framework on the other hand, a quantum sub-system enters an agent's lab only once. Many cryptographic protocols involve more than a single round of operations. In order to model multi-round protocols in the process matrix formalism, for example where two agents alternatively perform operations at different times on some states and exchange information, one would have to model a single agent, Alice as n different agents one for each round of the protocol, such that each agent acts only once on the states she receives. For protocols with larger number of agents and many rounds, the process matrix approach would be quite ineffective as one would need to keep track of many unnecessary inputs and outputs (corresponding to the additional agents) in the corresponding process matrix and the matrix itself grows in size.

Further, the causal boxes framework models superpositions of different number of messages as seen in Section 4.2.5. This in particular allows superpositions of sending "no message" (i.e., sending the vacuum state $|Omega\rangle$) and sending "one message". This would be required for modelling quantum cryptographic protocols where a party may chose to send a message or not send any message to another party depending (coherently) on the value of a control qubit.

Studying cryptographic applications of indefinite causal structures can provide an operational method for understanding the properties of physical causal structures. This would involve investigating questions such as: Which causal structures provide an operational advantage over others and in what kind of (cryptographic) tasks? What is the physical principle governing these causal structures that make them more useful for certain tasks?

4.2.7 Quantum causal models and causal discovery

The process matrix framework has been used for quantum causal modelling [10] and in the first quantum causal discovery algorithm [12]. As discussed in the introduction, in a quantum causal model, one has a number of nodes represented by "quantum systems" and directed edges or "causal mechanisms" connecting them. In addition, a quantum causal model must also provide a description of how these systems and mechanisms change under intervention and how one can predict such changes conditioned on a given intervention [9–11]. In the process matrix framework, the local laboratories can be viewed as the nodes and the channels appearing in the process matrix which connect different labs can be seen as the mechanisms and a framework for quantum causal modelling based on process matrices is presented in [10]. One can already get a flavour of this in the examples of Section 3.2.3 which are taken from this work. Further, [8] shows that classical causal discovery algorithms fail to satisfactorily explain quantum causal relations in the light of Bell's Theorem which creates the need for novel quantum causal discovery algorithms. Process matrices have been used to build the first quantum causal discovery algorithm [12]. At this stage, it is not completely clear how to use causal boxes in quantum causal modelling and causal discovery since the framework has a very different structure. However, there seems to be no fundamental limitation in the framework that does not allow its efficient use in such applications. In fact, the quantum causal model [10] only explicitly describes causally separable processes and causal discovery algorithm [12] can also only be applied to causally separable processes. Causal boxes can model causally separable processes which are known to be physically implementable. Thus, it should be possible to extend the methods of [10, 12] to the causal box framework. One can then check if the framework is suitable for causal modelling and causal discovery of indefinite causal structures such as the quantum switch. To the best of our knowledge, there is no known algorithm for the causal discovery of indefinite causal structures.

4.2.8 Quantum complexity

The problem of calculating the complexity of a circuit is an important one, but is far from trivial. As we noted in Section 1.4, the quantum switching operation between two unitaries when written out as a quantum circuit has at least one of the unitaries appearing twice (Figure 1.3). However, in the physical implementation (Figure 1.2), each unitary is applied only once. In fact, for the task of switching between n such unitaries, this difference between the number of gates appearing in the circuit drawing ($O(n^2)$) versus the number of gates actually applied ($O(n)$) grows much larger [29]. Thus, in the case where a superposition of ordered circuits is actually implemented (such as the quantum switch), merely counting the number of gates appearing in the circuit representation will not provide a correct estimate of the complexity because not all the gates are actually applied (some are applied to the vacuum state i.e., to "nothing"). However, performing a measurement to find out which gates where actually applied would destroy the coherence of the whole process. These observations reveal that evaluating the complexity of physically implementable quantum process is itself a large open question. In principle, this question could be investigated within both the causal boxes and process matrix frameworks. Among other things, such an analysis would involve superpositions of the vacuum state with other non-trivial quantum states (to model gates in a superposition of being applied and not). The process matrix framework in its original form [16] can not model such superpositions and one may need to generalise the framework to include such superpositions for example, by modelling the input and output spaces L_I and L_O of a lab L as Fock spaces instead of Hilbert spaces.

4.2.9 Definitions of causality

Another point of comparison between the causal box and process matrix frameworks is in their definitions of "causality". In the process matrix framework, causality is defined at the level of probability distributions where causal inequalities can be used to differentiate between *causal* and *non-causal* distributions. This definition of causality is "classical" i.e., it is formulated entirely at the level of classical settings and outcomes of agents. However, it is "non-classical" at the level of space-time structure since it makes no reference to an underlying space-time. The causality definition for causal boxes on one hand, appears more general since it makes no reference to specific inputs or outputs to the causal box (which may be classical or quantum) but on the other hand, appears less general because it appeals only to the fixed background space-time structure, $\mathcal{T}$ over which the causality function (Definition 2.2.2) is defined.

4.3 A summary of open questions

From the comparison and general discussion of the previous sections, a number of open questions are evident, and we summarise them here.

1. **Characterising the set of physical causal structures:** Process matrices were shown to be a strict subset of two-time states in [17] which provided a physical interpretation for all process matrices namely that they would arise naturally in a quantum world with post-selection. However, neither causal boxes nor process matrices are a strict subset of the other. Post-quantum systems arising in theories with fixed global ordering (Bell scenario), such as the PR box can be modelled with the causal boxes framework but not within the process matrix framework. While post-quantum systems arising in theories with no fixed global ordering, such as those which violate causal inequalities can be described within the process matrices framework but not within the causal boxes framework. Neither the former nor the latter are known to have physical implementation. Further, all physical processes with known physical implementations can be modelled within both frameworks. Exactly characterising the set of processes in the intersection of the two frameworks and identifying the basic property satisfied by all processes in this subset would provide a better understanding of the properties of physical causal structures. Thus, comparing these two frameworks goes beyond merely pin pointing the advantages and disadvantages of each framework since it would also be an important step towards tackling some of the big open questions in quantum causality.

2. **Causal modelling/discovery of indefinite causal structures:** The presently known quantum causal models [9, 10] and causal discovery methods [12, 13] can only be applied to specific cases of definite causal orders and can not handle any kind of superpositions of orders. Even these simple causal structures are fundamentally different in the quantum and classical cases as implied by Bell's theorem ([8]). The existing models are already a great progress for quantum causality because they provide a basic understanding of the notion of cause that governs quantum systems. However, the question of how one can generalise quantum causal models to superpositions of orders still remains open and it would be interesting to investigate if causal boxes could be useful for this purpose.

3. **Modelling superpositions of space-time with causal boxes:** As noted in Section 4.2.2, the causal boxes framework with its partially ordered structure, $\mathcal{T}$ cannot model superpositions of space-time structures. It would be interesting to see how the framework could be generalised, possibly by allowing for a causal box to be defined not over a fixed structure $\mathcal{T}$ but over a set of such partially ordered sets, each corresponding to a possible space-time geometry.

4. **Systems limited by relativistic causality alone:** Another area that could be explored with causal boxes is to examine how the framework could be generalised to include post-quantum systems constrained by special relativity alone [53]. This would have applications in post-quantum cryptographic protocols where adversaries are limited by relativistic causality alone [53]. As shown in Section 4.2.4, the causality conditions of the causal box framework are stronger than what is required by relativistic causality alone [53] since space-like separated parties in the framework always generate the "stronger" non-signalling correlations, which are only sufficient (but not necessary) for relativistic causality. As noted in Section 4.2.4, this would involve suitably relaxing Condition 2.12a or Definition 2.2.2.

5. **Quantum complexity:** As noted in Section 4.2.8, the question of evaluating the quantum complexity of processes involving a superposition of arbitrary quantum circuits still remains open. Given that merely counting the number of gates appearing in the circuit representation or performing a measurement to see which gates are actually applied would not give correct results, a novel method for achieving this is still lacking. Studying quantum complexity is crucial for quantum computing and allows us to talk about operational advantages provided by quantum processes over classical ones in solving certain information processing tasks (for example, see [28, 29]).

6. **Modelling agents as quantum systems:** In a theory involving quantum systems that allows agents to measure and operate on them, there is no reason why agents themselves should not be viewed as quantum systems that can be measured or operated upon by other agents. In such Wigner's friend [55] type scenarios, the probabilities assigned by different agents for the same set of events need not always be compatible with a single global probability distribution [56]. The process matrix framework allows only for process matrices that give valid global probability distributions according to the rule (3.5). It would be interesting to study if either of these frameworks allow for agents to be modelled as quantum systems themselves and if not, which features prevent them from doing so. After all, if causality allows us to consider situations where planets can be in quantum superpositions, then why not human beings?

Bibliography

[1] Vilasini, V., Portmann, C. & del Rio, L. Composable security in relativistic quantum cryptography. *New Journal of Physics* (2019). URL https://iopscience.iop.org/article/10.1088/1367-2630/ab0e3b.

[2] Bell, J. On the Einstein-Podolsky-Rosen paradox. *Physics* **1**, 195–200 (1964). URL https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.115.250401.

[3] Giustina, M. *et al.* Significant-Loophole-Free Test of Bell's Theorem with Entangled Photons. *Physical Review Letters* **115**, 250401 (2015). URL https://link.aps.org/doi/10.1103/PhysRevLett.115.250401.

[4] Hensen, B. *et al.* Loophole-free Bell inequality violation using electron spins separated by 1.3 kilometres. *Nature* **526**, 682–686 (2015). URL https://www.nature.com/articles/nature15759.

[5] Shalm, L. K. *et al.* Strong Loophole-Free Test of Local Realism. *Physical Review Letters* **115**, 250402 (2015). URL https://link.aps.org/doi/10.1103/PhysRevLett.115.250402.

[6] Pearl, J. & Judea. *Causality : models, reasoning, and inference* (Cambridge University Press, 2000). URL http://dl.acm.org/citation.cfm?id=331969.

[7] Spirtes, P., Glymour, C. N. & Scheines, R. *Causation, prediction, and search.* (Springer, New York, NY, 2000). URL https://link.springer.com/book/10.1007%2F978-1-4612-2748-9.

[8] Wood, C. J. & Spekkens, R. W. The lesson of causal discovery algorithms for quantum correlations: causal explanations of Bell-inequality violations require fine-tuning. *New Journal of Physics* **17**, 33002 (2015). URL https://iopscience.iop.org/article/10.1088/1367-2630/17/3/033002.

[9] Allen, J.-M. A., Barrett, J., Horsman, D. C., Lee, C. M. & Spekkens, R. W. Quantum Common Causes and Quantum Causal Models. *Physical Review X* **7**, 031021 (2017). URL http://link.aps.org/doi/10.1103/PhysRevX.7.031021.

[10] Costa, F. & Shrapnel, S. Quantum causal modelling. *New Journal of Physics* **18**, 63032 (2016). URL https://iopscience.iop.org/article/10.1088/1367-2630/18/6/063032.

[11] Leifer, M. S. & Spekkens, R. W. Towards a formulation of quantum theory as a causally neutral theory of Bayesian inference. *Physical Review A* **88**, 052130 (2013). URL https://link.aps.org/doi/10.1103/PhysRevA.88.052130.

[12] Giarmatzi, C. & Costa, F. A quantum causal discovery algorithm. *npj Quantum Information* **4** (2018). URL https://www.nature.com/articles/s41534-018-0062-6.

[13] Pienaar, J. & Brukner, Č. A graph-separation theorem for quantum causal models. *New Journal of Physics* **17**, 73020 (2015). URL https://iopscience.iop.org/article/10.1088/1367-2630/17/7/073020.

[14] Aharonov, Y., Bergmann, P. G. & Lebowitz, J. L. Time Symmetry in the Quantum Process of Measurement. *Physical Review* **134**, B1410–B1416 (1964). URL https://link.aps.org/doi/10.1103/PhysRev.134.B1410.

[15] Hardy, L. Probability Theories with Dynamic Causal Structure: A New Framework for Quantum Gravity (2005). URL http://arxiv.org/abs/gr-qc/0509120.

[16] Oreshkov, O., Costa, F. & Brukner, Č. Quantum correlations with no causal order. *Nature Communications* **3**, 1092 (2012). URL https://www.nature.com/articles/ncomms2076.

[17] Silva, R. *et al.* Connecting processes with indefinite causal order and multi-time quantum states. *New Journal of Physics* **19**, 103022 (2017). URL https://doi.org/10.1088%2F1367-2630%2Faa84fe.

[18] Portmann, C., Matt, C., Maurer, U., Renner, R. & Tackmann, B. Causal Boxes: Quantum Information-Processing Systems Closed under Composition. *IEEE Transactions on Information Theory* **63**, 3277–3305 (2017). URL http://ieeexplore.ieee.org/document/7867830/.

[19] Zych, M., Costa, F., Pikovski, I. & Brukner, C. Bell's Theorem for Temporal Order (2017). URL http://arxiv.org/abs/1708.00248.

[20] Chiribella, G., D'Ariano, G. M., Perinotti, P. & Valiron, B. Quantum computations without definite causal structure. *Physical Review A* **88**, 022318 (2013). URL https://link.aps.org/doi/10.1103/PhysRevA.88.022318.

[21] Araújo, M. *et al.* Witnessing causal nonseparability. *New Journal of Physics* **17**, 102001 (2015). URL https://iopscience.iop.org/article/10.1088/1367-2630/17/10/102001.

[22] Branciard, C., Araújo, M., Feix, A., Costa, F. & Brukner, Č. The simplest causal inequalities and their violation. *New Journal of Physics* **18**, 13008 (2016). URL https://iopscience.iop.org/article/10.1088/1367-2630/18/1/013008.

[23] Araújo, M., Feix, A., Navascués, M. & Brukner, Č. A purification postulate for quantum mechanics with indefinite causal order. *Quantum* **1**, 10 (2016). URL https://quantum-journal.org/papers/q-2017-04-26-10/.

[24] Pienaar, J. Causality in the Quantum World A new model extends the definition of causality to quantum-mechanical systems (2017). URL https://physics.aps.org/articles/v10/86.

[25] Reichenbach, H. *The direction of time* (Univ. of California Press, Berkeley - Los Angeles, 1956).

[26] Rubino, G. *et al.* Experimental verification of an indefinite causal order. *Science Advances* **3** (2017). URL http://advances.sciencemag.org/content/3/3/e1602589.

[27] Procopio, L. M. *et al.* Experimental superposition of orders of quantum gates. *Nature Communications* **6**, 7913 (2015). URL https://www.nature.com/articles/ncomms8913.

[28] Colnaghi, T., D'Ariano, G. M., Facchini, S. & Perinotti, P. Quantum computation with programmable connections between gates. *Physics Letters A* **376**, 2940 – 2943 (2012). URL http://www.sciencedirect.com/science/article/pii/S0375960112009280.

[29] Araújo, M., Costa, F. & Brukner, Č. Computational Advantage from Quantum-Controlled Ordering of Gates. *Physical Review Letters* **113**, 250402 (2014). URL https://link.aps.org/doi/10.1103/PhysRevLett.113.250402.

[30] Chiribella, G., D'Ariano, G. M. & Perinotti, P. Theoretical framework for quantum networks. *Physical Review A* **80**, 022339 (2009). URL https://link.aps.org/doi/10.1103/PhysRevA.80.022339.

[31] Aharonov, Y. & Vaidman, L. Complete description of a quantum system at a given time. *Journal of Physics A: Mathematical and General* **24**, 2315 (1991). URL https://iopscience.iop.org/article/10.1088/0305-4470/24/10/018.

[32] Silva, R. *et al.* Pre- and postselected quantum states: Density matrices, tomography, and kraus operators. *Physical Review A* **89**, 012121 (2014). URL https://link.aps.org/doi/10.1103/PhysRevA.89.012121.

[33] Gutoski, G. On a measure of distance for quantum strategies. *Jounal of Mathematical Physics* **53**, 032202 (2012). URL https://aip.scitation.org/doi/10.1063/1.3693621.

[34] Hardy, L. The operator tensor formulation of quantum theory. *Philosophical Transactions of the Royal Society of London A: Mathematical, Physical and Engineering Sciences* **370** (2012). URL http://rsta.royalsocietypublishing.org/content/370/1971/3385.

[35] Friis, N., Dunjko, V., Dür, W. & Briegel, H. J. Implementing quantum control for unknown subroutines. *Physical Review A* **89**, 030303 (2014). URL https://link.aps.org/doi/10.1103/PhysRevA.89.030303.

[36] Thompson, J., Modi, K., Vedral, V. & Gu, M. Quantum plug n' play: modular computation in the quantum regime. *New Journal of Physics* **20**, 013004 (2018). URL https://doi.org/10.1088%2F1367-2630%2Faa99b3.

[37] Araújo, M., Feix, A., Costa, F. & Brukner, Č. Quantum circuits cannot control unknown operations. *New Journal of Physics* **16**, 93026 (2014). URL https://iopscience.iop.org/article/10.1088/1367-2630/16/9/093026.

[38] Zhou, X.-Q. *et al.* Adding control to arbitrary unknown quantum operations. *Nature Communications* **2**, 413 (2011). URL https://www.nature.com/articles/ncomms1392.

[39] Nielsen, M. A. & Chuang, I. L. *Quantum computation and quantum information* (Cambridge University Press, 2010). URL http://www.cambridge.org/ch/academic/subjects/physics/quantum-physics-quantum-information-and-quantum-computation/quantum-computation-and-quantum-information-10th-anniversary-edition?format=PB{&}isbn=9781107002173{#}1JihLXCbgpiGkusk.97.

[40] Maurer, U. & Renner, R. Abstract Cryptography. In Chazelle, B. (ed.) *The Second Symposium on Innovations in Computer Science, ICS 2011*, 1–21 (Tsinghua University Press, 2011).

[41] Brunner, N., Cavalcanti, D., Pironio, S., Scarani, V. & Wehner, S. Bell nonlocality. *Reviews of Modern Physics* **86**, 419–478 (2014). URL https://link.aps.org/doi/10.1103/RevModPhys.86.419.

[42] Clauser, J. F., Horne, M. A., Shimony, A. & Holt, R. A. Proposed Experiment to Test Local Hidden-Variable Theories. *Physical Review Letters* **23**, 880–884 (1969). URL https://link.aps.org/doi/10.1103/PhysRevLett.23.880.

[43] Oreshkov, O. & Giarmatzi, C. Causal and causally separable processes. *New Journal of Physics* **18**, 93020 (2016). URL https://iopscience.iop.org/article/10.1088/1367-2630/18/9/093020.

[44] Pironio, S. All Clauser-Horne-Shimony-Holt polytopes. *Journal of Physics A: Mathematical and Theoretical* **47**, 424020 (2014). URL https://iopscience.iop.org/article/10.1088/1751-8113/47/42/424020.

[45] Cirel'son, B. S. Quantum generalizations of Bell's inequality. *Letters in Mathematical Physics* **4**, 93–100 (1980). URL http://link.springer.com/10.1007/BF00417500.

[46] Larsson, J.-Å. Loopholes in bell inequality tests of local realism. *Journal of Physics A: Mathematical and Theoretical* **47**, 424003 (2014). URL https://doi.org/10.1088%2F1751-8113%2F47%2F42%2F424003.

[47] Abbott, A. A., Giarmatzi, C., Costa, F. & Branciard, C. Multipartite causal correlations: Polytopes and inequalities. *Physical Review A* **94**, 032131 (2016). URL https://link.aps.org/doi/10.1103/PhysRevA.94.032131.

[48] Horodecki, M., Horodecki, P. & Horodecki, R. Separability of mixed states: necessary and sufficient conditions. *Physics Letters A* **223**, 1 – 8 (1996). URL http://www.sciencedirect.com/science/article/pii/S0375960196007062.

[49] Terhal, B. M. Bell inequalities and the separability criterion. *Physics Letters A* **271**, 319 – 326 (2000). URL http://www.sciencedirect.com/science/article/pii/S0375960100004011.

[50] Chiribella, G. Perfect discrimination of no-signalling channels via quantum superposition of causal structures. *Physical Review A* **86**, 040301 (2012). URL https://link.aps.org/doi/10.1103/PhysRevA.86.040301.

[51] Popescu, S. & Rohrlich, D. Quantum nonlocality as an axiom. *Foundations of Physics* **24**, 379–385 (1994). URL http://link.springer.com/10.1007/BF02058098.

[52] Hardy, L. Quantum Theory From Five Reasonable Axioms (2001). URL http://arxiv.org/abs/quant-ph/0101012.

[53] Horodecki, P. & Ramanathan, R. Relativistic Causality vs. No-Signaling as the limiting paradigm for correlations in physical theories (2016). URL http://arxiv.org/abs/1611.06781.

[54] Portmann, C. & Renner, R. Cryptographic security of quantum key distribution (2014). URL http://arxiv.org/abs/1409.3525.

[55] Wigner, E. P. *Remarks on the Mind-Body Question* (Indiana University Press, Bloomington, Indiana, 1967). URL https://link.springer.com/chapter/10.1007%2F978-3-642-78374-6_20.

[56] Frauchiger, D. & Renner, R. Quantum theory cannot consistently describe the use of itself. *Nature Communications* **9**, 3711 (2018). URL https://www.nature.com/articles/s41467-018-05739-8.

Appendix

A Licence information

In this report, we have used certain figures, definitions and examples from published papers to supplement the literature review. We have provided the necessary citations wherever such content has been used. Here we provide details of the official licenses secured from the respective publishers that permits us to do so.

License for [10, 21, 22]

Works [10,21,22] are covered by a Creative Commons Attribution 3.0 Unported licence. It allows for reproducing, adapting and reviewing parts of the works for thesis/dissertation purposes, with due citations. The licence information is available at
https://creativecommons.org/licenses/by/3.0/legalcode.

License for [18]

The public licence for reproduction/adaptation (with due citations) of the content of the original work [18] in theses and dissertations is obtained from
http://ieeexplore.ieee.org/document/7867830/. It is shown below.

Copyright Clearance Center RightsLink®

Home | Account Info | Help

IEEE Requesting permission to reuse content from an IEEE publication

Title: Causal Boxes: Quantum Information-Processing Systems Closed Under Composition
Author: Christopher Portmann
Publication: Information Theory, IEEE Transactions on
Publisher: IEEE
Date: May 2017

Logged in as:
Vilasini V
Account #:
3001189293
LOGOUT

Thesis / Dissertation Reuse

The IEEE does not require individuals working on a thesis to obtain a formal reuse license, however, you may print out this statement to be used as a permission grant:

Requirements to be followed when using any portion (e.g., figure, graph, table, or textual material) of an IEEE copyrighted paper in a thesis:

1) In the case of textual material (e.g., using short quotes or referring to the work within these papers) users must give full credit to the original source (author, paper, publication) followed by the IEEE copyright line � 2011 IEEE.
2) In the case of illustrations or tabular material, we require that the copyright line � [Year of original publication] IEEE appear prominently with each reprinted figure and/or table.
3) If a substantial portion of the original paper is to be used, and if you are not the senior author, also obtain the senior author�s approval.

Requirements to be followed when using an entire IEEE copyrighted paper in a thesis:

1) The following IEEE copyright/ credit notice should be placed prominently in the references: � [year of original publication] IEEE. Reprinted, with permission, from [author names, paper title, IEEE publication title, and month/year of publication]
2) Only the accepted version of an IEEE copyrighted paper can be used when posting the paper or your thesis on-line.
3) In placing the thesis on the author's university website, please display the following message in a prominent place on the website: In reference to IEEE copyrighted material which is used with permission in this thesis, the IEEE does not endorse any of [university/educational entity's name goes here]'s products or services. Internal or personal use of this material is permitted. If interested in reprinting/republishing IEEE copyrighted material for advertising or promotional purposes or for creating new collective works for resale or redistribution, please go to http://www.ieee.org/publications_standards/publications/rights/rights_link.html to learn how to obtain a License from RightsLink.

If applicable, University Microfilms and/or ProQuest Library, or the Archives of Canada may supply single copies of the dissertation.

BACK ��� CLOSE WINDOW