Quantum Causal Structure

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To my parents, Richard and Regine.

In gratitude for their unconditional love and support
on my travels, in physics and otherwise.

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Albeit an obvious observation, given the interdependent nature of my existence, the few sensible things I have thought and said (in my thesis or elsewhere) can hardly be attributed to me alone — for the *causes* and conditions are always myriad.

Relevant publications and statement of authorship

This thesis is largely based on the following three publications:

(1) "Quantum Causal Models", J. Barrett, R. Lorenz and O. Oreshkov, arXiv:1906.10726 [quant-ph], (2019). (Ref. [1] in the bibliography.)

(2) "Causal and compositional structure of unitary transformations", R. Lorenz and J. Barrett, arXiv:2001.07774 [quant-ph], (2020). (Ref. [2] in the bibliography.)

(3) "Cyclic Quantum Causal Models", J. Barrett, R. Lorenz and O. Oreshkov, arXiv:2002.12157 [quant-ph], (2020). (Ref. [3] in the bibliography.)

Any content, idea or result in this thesis that is not also contained in these publications or otherwise due to myself, has been referenced appropriately, to the best of my knowledge. The above three pieces are joint work with my supervisor Jonathan Barrett and Ognyan Oreshkov, with the exception of the second work in Ref. [2], which was done together with only J. Barrett. The following outlines very roughly where my main contributions lie.

Chapter 4 mainly presents definitions and concepts common to all three publications. I was originally introduced to this approach to quantum causal structure by my supervisor Jonathan Barrett, following on from the preceding work by him and other authors in Ref. [4]. These ideas were sharpened and generalised over the course of the past three years by all three of us.

Chapter 5 presents the joint work from Ref. [1]. The main results come in two groups. First, there is the content of Sec. 5.2. The main results here are Thm. 5.1, in the proof of which I played a leading role, and Thm. 5.2, which is genuine joint work by all authors, with crucial ideas to fix an issue with my first formalisation of our ideas for the proof coming from my supervisor. Second, the proofs of the main theorems in Secs. 5.5 and 5.6 were largely due to me, but improved jointly. As for the final formulation of the notion of quantum relative independence from Sec. 5.4 and the formulation of various operational statements across Secs. 5.4-5.6, my supervisor played a leading role. The proofs related to these concepts were done jointly.

Chapter 6 presents the joint work with J. Barrett from Ref. [2]. The first main result (Thm. 6.2) was first conjectured by my supervisor and he played a leading role in its proof. Concerning the proofs of all other results and the way the work took shape, I then played a leading role. The final presentation was refined together.

Chapter 7 presents the joint work from Ref. [3]. This chapter's value, above all, is a conceptual one. It presents new ideas that were initiated by myself and O. Oreshkov and then further refined and explored jointly by all authors. The observation in Sec. 7.5.1 is due to O. Oreshkov, the one in Sec. 7.5.2 due to me. The few minor technical results in Sec. 7.6 were done by myself. The results from Ref. [3], in the proof of which I was not much involved, are not presented in this thesis.

Regarding the presentation of the material in the three publications, which of course heavily influenced the presentation of the work in this thesis, I wrote the initial drafts for all three manuscripts, which then, especially for Ref. [1] and Ref. [3], were considerably changed and improved by my co-authors.

Abstract

Quantum theory challenges our intuitions of causality, as manifest in the existence of Bell non-local correlations. The latter seem to falsify Reichenbach's common cause principle and evade causal explanations within the classical causal model framework developed in recent decades. But could quantum correlations be explained in causal, albeit *quantum causal* terms? Even if one embraces a revised causal relation, challenges of our intuitions seem to persist — for instance, 'quantum indefinite causal order' of events being conceivable and intensely studied.

This thesis hopes to contribute to our understanding of how causal reasoning can be maintained, in a rigorous manner, in light of quantum theory. Inspired by the work of Allen *et al.* [Phys. Rev. X 7, 031021 (2017)], a definition of *quantum causal relations* is given in terms of influence in underlying unitary transformations. The notion of *quantum causal structure* that ensues is then explored in three, closely related directions.

First, a *quantum causal model* framework is presented that generalises classical causal models and allows causal explanations of quantum processes, assuming that a definite causal order does exist. Amongst other things, notions of 'quantum conditional independence' are presented and generalisations of core classical theorems, such as the d-separation theorem, are derived.

Second, the thesis studies how causal structure of unitary transformations can be understood in terms of their *compositional structure.* The results here reveal how causal structure is closely associated with the interplay between direct sums and direct products of Hilbert spaces. An extension of quantum circuit diagrams is introduced to visualise the found 'causal decompositions' of unitaries.

Third, a generalisation of quantum causal models to *cyclic causal structure* is proposed, to analyse processes that feature indefinite causal order. The idea is illustrated through analysing well-known examples of such processes and some first results are presented.

Contents

Chapter 1

Introduction

Usually, shortly after pressing the switch of a kettle, the water is boiling and ready to make the ubiquitous English cup of tea. Of course, we know *why* this is the case — the kettle was designed to have a mechanism through which, as we are happy to assert, the pressing of the switch *causes* the heating of the water. In contrast, on most days that the sales of umbrellas in London are particularly high, the number of daily visitors to Hyde park is particularly low. We would not be led to believe that either causes the other, but rather assert that the culprit is rain as a common cause.

Having this causal understanding changes how we engage with the world; whether it is knowing how long before a friend's arrival we need to 'put the kettle on', or whether we had better stay indoors that afternoon. However, it is not only our everyday life, but also science, that is inseparable from thinking in causal terms. The very business of a scientific discipline often appears to be developing a causal understanding of the phenomena under study. For instance, a good theory about ocean currents is one that allows an understanding of the mechanisms that govern them — the 'causal mechanisms' — for only then do we feel we really understand a phenomenon, and can anticipate what happens if some of the parameters are altered. Scientific practice also relies on causal thinking at the methodological level. That two experiments can be regarded as independent sources of evidence for a hypothesis appears as reliant on a basic causal assessment of the situation.

So, if causal reasoning is so basic, how does one infer causation from observations, seeing as observations constitute the basis of the empirical sciences? What of the phrase we all have been educated to cherish — 'correlation does not imply causation'? Indeed, the fact that there are two correlated variables is the same in both examples at the beginning and to that extent, just given statistics about the respective variables, they are indistinguishable. Nonetheless, in the first example of the kettle we would assert a causal link between pressing the button and the water boiling, whereas in the second, we do not buy into a causal link between umbrella sales and visitor numbers in Hyde park, but rather assert a common cause. While in these examples it may be uncontroversial which different causal explanations we regard as plausible, scientific practice needs a principled methodology.

To this end, it is necessary to make precise how claims about the causal relations of variables and statistical statements about them relate to one another. In the first half of the last century Hans Reichenbach thought a great deal about this relation (see, e.g., Refs. [5–7]) and the intuitive essence of his famous *common cause principle* is simple and omnipresent in science: if two variables are correlated, but none is the cause of the other, then there ought to exist a common cause in the past, conditional on which the original variables are rendered statistically independent.

However, only with the advent of *causal models*, pioneered by Peter Spirtes, Clark Glymour and Richard Scheines (see Ref. [8]) and Judea Pearl and his collaborators (see Ref. [9]), was a general framework for causal reasoning obtained, that, amongst other things, moved the problem of causal inference into the realm of scientific methodology. It facilitated the development of 'causal discovery algorithms', which spell out in a principled way under which assumptions the causal structure *can* be inferred from observational data. In a causal model the causal structure is typically represented by a *directed acyclic graph* (DAG), where arrows represent causal relationships between the variables and the DAG as a whole is part of the causal explanation of the probability distribution over the same variables. The reason humans care so much about causal relations is succinctly expressed in Pearl's metaphor of the three rungs for the advantage of causal reasoning [10]: at a first rung, statistics from observations alone only allow predictions for future observations, such as the probability to observe $B = b$, given that one has observed $A = a$; while with additional and increasingly detailed causal knowledge at rungs two and three, the framework of causal models allows us to answer entirely different kinds of questions such as questions of an interventional nature — what would happen to variable B if one intervened and changed variable A — or of a counterfactual nature — what would have happened to B, had A been observed to be different. Causal models have found widespread application in fields ranging from AI and medicine to economics and sociology [10].

A natural question to ask is what should one make of all these developments from the perspective of physics, in particular in light of quantum theory? Can we uphold our natural inclination to understand the physical world in causal terms in a similarly precise way and, in particular, give causal explanations of the correlations that can arise in experiments involving quantum systems?

Intuitively speaking, if quantum physics is incompatible with a description in terms of variables that have pre-existing values prior to measurement, then it seems at odds with hoping to give causal explanations of quantum correlations with causal models, where causal relata are classical variables. Indeed, one of the seminal no-go theorems, that make precise in which sense one can claim such a feature of quantum theory — Bell's theorem [11, 12] — precisely rules out the explanation of Bell-inequality violating correlations in terms of a common cause variable in the past. Importantly, other conclusions from Bell's theorem that are aimed at saving a 'picture of classical variables with definite values' — such as retrocausal explanations, superluminal signalling or superdeterminism — were shown to lead to causal model explanations that are necessarily fine-tuned [13]. So, the answer to the above question is 'no'; insofar as the framework of *classical* causal models cannot generally provide satisfactory causal explanations of quantum correlations. The obvious question then must be: if not in terms of classical causal structure, can quantum correlations be explained in terms of *quantum* causal structure?

We shall return to this question momentarily. Doing so, will in particular raise the question of what exactly 'quantum causal structure' is supposed to be. The past three decades, and especially the past 10 years, have seen a surge of research on 'causality' in quantum theory. Most of it is *not* concerned with giving explanations à la Reichenbach or causal models, and studies a range of different questions, but still derives from an intuition of and interest in causality of some kind or other. The below touches on only a tiny fraction of such works.

One common perspective is to think of a set of quantum systems as being embedded into a fixed space-time and to then study which kind of quantum channels (completely positive trace-preserving maps), describing the evolution of these systems, is in keeping with relativity. In particular, one may then ask which channels do not lead to the possibility of signalling between space-like separated systems and which no-signalling correlations they generate. Conversely, where there is possible signalling between two systems, one may ask whether this is compatible with a finite speed of propagation and that the channel has an implementation with a 'sequence of local interactions' as a quantum circuit diagram may be taken to represent. See, e.g., Refs. [14–18] for a small selection of works in this spirit.

In the context of the framework of operational probabilistic theories [19] and categorical quantum mechanics [20–25], 'causality' was formalised as a property of processes which could be paraphrased as 'no signalling back from the future' and played an important role in studying the compositional structure of quantum theory and in axiomatisations of quantum theory [26–28]. The link of this notion of 'causality' with 'relativistic causality', that is, the above mentioned constraints on signalling through a quantum channel, as well as with other concepts often associated with causality such as determinism, was elucidated in Refs. [23, 29–31].

Another formalism that is built around the causal intuitions about a 'quantum network' is that of quantum combs [32], which looks at quantum circuits from a higher-order perspective and studies how circuits can be transformed into other circuits, with quantum circuit optimisation being one problem for which it is useful. A general framework for studying the quantum information-processing properties of systems through modelling them as 'causal boxes' was developed by Portmann *et al.* in Ref. [33]. The study of generalised Bell inequalities in more complex causal scenarios than the original Bell scenario has also been widely examined (see, e.g., Refs. [13, 34–39]).

Now, an important distinction is that between *spacio-temporal* relations and *causal* relations. Our concept of causality often seems inseparable from events occurring in, or systems existing in space-time. However, completely independently from the kinds of systems, quantum or not, it is important to note that spacio-temporal relations in a fixed background space-time impose constraints on what *can possibly* be causally related to what, but does not tell us what *actually* is causally related to what. If two quantum systems are time-like separated, then all we know is that it is not contradictory to suppose they might be causally related. The sense of *quantum causal structure* this thesis has in mind is causal structure as the set of relations of what actually is causally related to what. One can always ask whether a particular way of placing systems in a space-time is consistent with some asserted causal relations, but, for the most part, this thesis will not concern itself with this.

Nonetheless, even if not primarily concerned with spacio-temporal relations, one aspect of our intuition surely must persist (one would think) — whatever the causal relations are, they always form a *causal order*, where loosely speaking, no influence is going in loops. However, this very intuition of a fixed causal order is challenged in the most hotly debated questions in quantum causality, a field concerned with *indefinite causal order*. Triggered by a number of groundbreaking works, motivation for such considerations comes from quantum gravity, as Hardy argued in Refs. [40, 41], and from considering the 'superposition of causal orders' in quantum circuits, controlled by another quantum system, as studied by Chiribella *et al.* in Ref. [42]. Oreshkov, Costa and Brukner in Ref. [43] then introduced the framework of *process matrices*, with which it is possible to describe any correlations between operations that can locally be described by quantum mechanics, while no assumption is made that, globally, the operations fit into any fixed causal order. Surprisingly, they discovered processes that are logically consistent, but indeed incompatible with any fixed causal order. Understanding the scope and the physical status of 'indefinite causality' is an extremely active area of research (see, e.g., Refs. [42, 44–72] for a selection, and the review in a later chapter).

With so much energy and thought devoted to the field of 'quantum causality', one might think it must be obvious and agreed what causal relations in the context of quantum systems are in the first place. While quantum causation is usually taken to be about 'signalling', we would like to argue that the notion of causal relations needs careful examination. The emergence of the field of indefinite causality makes it still more important to provide a solid foundation to the study of quantum causal relations.

Giving an account of the description of matter of affairs in terms of what actually is causally related to what, is what causal models are supposed to formalise and guide. This brings us back to the earlier conclusion of the inadequacy of classical causal models to understand Bell correlations and to the question whether a genuine quantum generalisation of the framework can be developed that similarly formalises the causal analysis of any set of quantum systems and the correlations they give rise to. A lot of effort has been put into the development of this (see, e.g., Refs. [4,34,35, 73–88]). These works agree on the use of DAGs for representing causal structure and that quantum systems are involved, however, there are otherwise large differences. A review of these approaches will be given later. Specifically, we will argue that they all, with the exception of the proposed definition by Allen *et al.* from Ref. [4], lack generality or do not meet desirable desiderata for a quantum causal model framework.

In order to provide a conceptually clear grounding for a quantum causal model framework and any talk about quantum causal structure, it is helpful to disentangle two steps:

(1) Define the quantum causal relation. This will have to be some 3-place relation of the form 'C is a direct cause of E given $\mathcal{M}$ if and only if some condition CR holds', that is, it has to say what sort of object C and E are, relative to what sort of data $\mathcal{M}$ causal relations are defined at all and what the causal connection is, i.e. which condition CR captures that C stands to E in a causal relationship.

(2) Develop a quantum causal model framework. This has to spell out, in particular, when and how to give causal explanations, in accordance with (1) and in a principled way, when the given data is not of the kind as demanded by $\mathcal{M}$.

Importantly, and as will be argued later, 'signalling through a quantum channel', or more generally 'through a quantum process' — the dominant intuition on quantum causation in the literature — does not provide a satisfactory basis for a definition of the form as in (1). A priori, it is of course conceivable that there is more than one consistent way of following an approach as sketched in the scheme of steps (1) and (2). However, none of the above cited works does this, with the mentioned work by Allen *et al.* in Ref. [4] again being the only exception. The spirit of the latter work is exactly such an approach and the core suggestion is, roughly speaking, to take causal relations between quantum systems as influence in underlying unitary evolution. On that basis, their main achievement consists in formulating a quantum generalisation of Reichenbach's common cause principle and deriving it as a theorem, as it were, rather than proposing it as an ad-hoc principle. Taking inspiration from the form of this principle, Ref. [4] then proposes a definition of a quantum causal model, without however similarly substantiating it with a theorem, and without much further exploration of that definition and the framework it leads to.

The content and structure of this thesis

What this thesis will undertake could be summarised as follows. First, following the suggestion from Ref. [4], it formalises the quantum causal relation and the corresponding most general notion of quantum causal structure of a set of quantum systems. Second, it fills the gap by formally going from above step (1) to step (2). Third, in what will form the main body of the thesis, it derives a series of results that explore quantum causal structure along several axes, including, but not restricted to the causal model perspective. This notion of quantum causal relations based on influence in unitary transformations by no means goes against the intuition of signalling between agents, but rather finds the latter to be a typical manifestation or expression of a causal connection.

One goal of the thesis is therefore to help establish a promising definition of quantum causal structure — promising insofar as it is conceptually and mathematically clear and facilitates new results that are of interest, regardless of whether or not one agrees with the above sketched scheme. These results concern for instance novel notions of 'quantum conditional independence', structural properties of unitary transformations and insights into the properties of processes with 'indefinite causal order'. However, this work will be restricted to the study of finite-dimensional quantum systems and no attempt is made to extend the ideas to a quantum field theoretic context.

The following outlines the structure and sets out more concretely what one can expect to find in this thesis.

After introducing some notation and necessary conventions in Chap. 2, Chapter 3 introduces the necessary background knowledge on which the thesis builds. In particular, it will give a summary of classical causal models with a focus on those aspects that will serve a pedagogical purpose in the quantum case. It will also summarise the prior work on quantum causal models, with a view to bringing out clearly why there were open questions concerning the establishment of a satisfactory definition, as claimed above.

Chapter 4 then constitutes the foundation of this whole thesis by presenting the definitions, which the subsequent chapters explore: the definition of the quantum causal relation and the induced notion of quantum causal structure relative to unitary transformations, and more generally, unitary processes. It will give some basic analysis of why this proposal is distinct and where the motivation stems from.

Chapter 5 is the first chapter with substantial results. It presents and explores a fully-fledged framework of *quantum causal models*, based on the proposal from Ref. [4]. It has two main parts, the first of which roots the framework in the definition of quantum causal structure as defined in Chap. 4 by proving a theorem to an analogous effect to the main result from Ref. [4] for the quantum common cause principle (see Sec. 5.2.3). In the second part it essentially explores consequences from causal structure at the level of non-unitary processes. This involves in particular the introduction of genuinely quantum versions of conditional independence in Sec. 5.4 and the derivation of quantum generalisations of some of the main theorems of the classical framework, namely, of the d-separation theorem in Sec. 5.5 and of the three rules of the do-calculus in Sec. 5.6. Finally, it makes some first observations about quantum causal inference in Sec. 5.7.3.

Seeing Chap. 5 as studying how causal structure, defined at the level of the underlying unitary processes, manifests itself 'at the higher level' in the properties of non-unitary processes, Chapter 6 can be seen as 'going down' and seeking to find a more fine-grained understanding of the causal mechanisms in unitary processes. It will do so by asking whether causal structure can be understood in compositional terms and first argue in Sec. 6.2 that compositional structure as expressible with ordinary circuit diagrams is not sufficient to this end. Section 6.3 will show that direct sum structures, and in particular its interplay with direct products, are crucial for a compositional understanding of causal structure. Section 6.4 will introduce a novel type of diagrams, *extended circuit diagrams*, to overcome the limitations of circuit diagrams and Sec. 6.6 will derive many results where the causal structure of a unitary map implies an extended circuit decomposition that makes the respective causal structure evident in situations where circuit diagrams cannot achieve this.

Chapter 7, the third main chapter, can be seen as the application of the ideas and insights from the preceding chapters to processes with 'indefinite causal order'. This naturally presents itself as exploring the case of the general definition of causal structure in Chap. 4 for when that is not a DAG, but a cyclic directed graph. This chapter will begin by first giving a brief introduction into the field of 'indefinite causal order' (see Sec. 7.1). Sections 7.2 and 7.3 will then introduce a generalisation of quantum causal models to *cyclic causal structure*, with prominent examples of such to be studied in Sec. 7.4. Section 7.5 will exemplify how the results on 'causal decompositions' from Chap. 6 lead to new insights on 'causally indefinite processes' and Sec. 7.7 will update quantum causal inference in light of the presented generalisations.

Finally, Chap. 8 will conclude the thesis by summarising the work and the open questions, and by sharing some final reflections.

Chapter 2

Notation and conventions

2.1 Classical variables

When considering random variables it is assumed throughout that they take values in sets of *finite cardinality*. A joint probability distribution over a set of n variables $\{X_1, \ldots, X_n\}$ is denoted $P(X_1, \ldots, X_n)$. For disjoint sets of variables X, Y and Z writing $P(X, Y, Z)$ has the obvious meaning. An expression like $P(X, Y|Z)$, apart from denoting a Bayesian conditional obtained from a joint distribution, will also be used to refer to a classical channel, that is, for every value z that the variable Z may take, the data specifies a probability distribution $P(X, Y|Z = z)$ over $X \times Y$, so that $P(X, Y|Z)$ defines a stochastic map. The context will always make clear how expressions like $P(X, Y|Z)$ are to be understood.

2.2 Quantum systems and the Choi-Jamiołkowksi isomorphism

The Hilbert space associated with a quantum system A is denoted $\mathcal{H}_A$ and throughout assumed to be of *finite dimension* d_A. The vector space of linear operators on $\mathcal{H}_A$ is denoted $\mathcal{L}(\mathcal{H}_A)$ and a state of system A, i.e. a trace-1, positive semi-definite operator in $\mathcal{L}(\mathcal{H}_A)$, is denoted ρ_A. For S a set of quantum systems, write $\mathcal{H}_S := \bigotimes_{A \in S} \mathcal{H}_A$ (the order of systems is left implicit).

A *completely positive* (CP) map $\mathcal{E} : \mathcal{L}(\mathcal{H}_A) \to \mathcal{L}(\mathcal{H}_B)$ is typically denoted with a curly letter and a trace-preserving CP map is referred to as a CPTP map, or interchangeably, a *quantum channel*, or just channel for short. A channel $\mathcal{U}$: $\mathcal{L}(\mathcal{H}_A) \to \mathcal{L}(\mathcal{H}_B)$ is called a unitary channel if and only if there exists a unitary map $U : \mathcal{H}_A \to \mathcal{H}_B$ such that $\mathcal{U}(\ \_\ ) = U(\ \_\ )U^\dagger$ (a unitary map U is not necessarily assumed to be an automorphism, but given by any linear map that defines a bijection between ortho-normal bases).

A very useful tool in quantum information theory, which will be made heavy use of in this thesis, is the *Choi-Jamiołkowksi* (CJ) isomorphism [89, 90] that allows the treatment of states of systems and channels between systems mathematically on an equal footing. Following Ref. [4] and consistently with Refs. [1–3], which this thesis is based on, a particular variant of the CJ isomorphism is used here. Given a CP map $\mathcal{E} : \mathcal{L}(\mathcal{H}_A) \to \mathcal{L}(\mathcal{H}_B)$ its CJ operator is defined as

$$\rho^{\mathcal{E}}_{B|A} := \sum_{i,j} \mathcal{E}\big(|i\rangle_A \langle j| \big) \otimes |i\rangle_{A^*} \langle j| \ , \tag{2.1}$$

where $\{|i\rangle_A\}$ is an orthonormal basis of $\mathcal{H}_A$, and $\{|i\rangle_{A^*}\}$ the corresponding dual basis. The way that $\rho^{\mathcal{E}}_{B|A} \in \mathcal{L}(\mathcal{H}_B \otimes \mathcal{H}^*_A)$ is defined to act on the dual of $\mathcal{H}_A$ allows for the representation of CP maps with CJ operators that are positive semi-definite and basis independent. In CJ representation the image of ρ_A under $\mathcal{E}$ becomes

$$\mathcal{E}(\rho_A) = \mathrm{Tr}_{AA^*}\big[\ \rho^{\mathcal{E}}_{B|A} \ \tau^{\mathrm{id}}_A \ \rho_A \ \big] \tag{2.2}$$

with the 'linking operator'

$$\tau^{\mathrm{id}}_A \ := \ \sum_{i,j} \ |i\rangle_{A^*} \langle j| \otimes |i\rangle_A \langle j| \ . \tag{2.3}$$

Using the short-hand notation $\overline{\mathrm{Tr}}_A[\ \_\ ] := \mathrm{Tr}_{AA^*}[\tau^{\mathrm{id}}_A \ \_]$ one can then write $\mathcal{E}(\rho_A) = \overline{\mathrm{Tr}}_A[\rho^{\mathcal{E}}_{B|A} \ \rho_A]$, which is reminiscent of $\sum_X P(Y|X)P(X)$, the image of a probability distribution $P(X)$ under the classical channel defined by $P(Y|X)$. Conversely, given any positive semi-definite operator $\alpha \in \mathcal{L}(\mathcal{H}_B \otimes \mathcal{H}^*_A)$, then $\mathcal{C}(\_) := \overline{\mathrm{Tr}}_A[\alpha \ \_]$ defines a CP map of the form $\mathcal{C} : \mathcal{L}(\mathcal{H}_A) \to \mathcal{L}(\mathcal{H}_B)$. Importantly, the CJ operator $\rho^{\mathcal{E}}_{B|A}$ represents a CPTP map if and only if $\mathrm{Tr}_B[\rho^{\mathcal{E}}_{B|A}] = \mathbb{1}_{A^*}$. For proofs and further facts about the CJ representation of channels see, for instance, Ref. [32].

Given the 1-to-1 correspondence between channels and their CJ operators, we will often write 'given a channel $\rho_{B|A}$' by stating the CJ operator and also suppress the superscript $\mathcal{E}$ unless there is ambiguity. Furthermore, given the correspondence between unitary channels $\mathcal{U}$ and the associated unitary map U between the underlying Hilbert spaces, we will use both $\rho^{U}_{B|A}$ and $\rho^{\mathcal{U}}_{B|A}$ for the CJ operator of the unitary channel.

A convention that will be used frequently (and was already employed in Eq. (2.2)) is writing products of the form $\rho_{D|AB} \ \rho_{E|BC}$ as a short-hand for the product of operators that are appropriately 'padded' with identity operators, i.e., it is short for $(\rho_{D|AB} \otimes \mathbb{1}_{EC^*})(\mathbb{1}_{DA^*} \otimes \rho_{E|BC})$.

2.3 Graphs and circuit diagrams

A *directed graph* G is given by a set V of vertices (also called nodes) and a set of arrows, formally given by a subset E of $V \times V$ such that G has an arrow $v \to w$ if and only if $(v, w) \in E$. Given a directed graph G a path of length n is a sequence of vertices $v_1, v_2, \ldots..., v_{n+1}$ such that there is an arrow between v_i and v_{i+1} (in either direction) for all $i = 1, .., n$. The path is called a directed path if for each $i = 1, .., n$ the arrow goes from v_i to v_{i+1} and it is a directed cycle if furthermore $v_1 = v_{n+1}$. A *directed acyclic graph* (DAG) is a directed graph that does not contain any directed cycle. See Fig. 2.1 for examples.

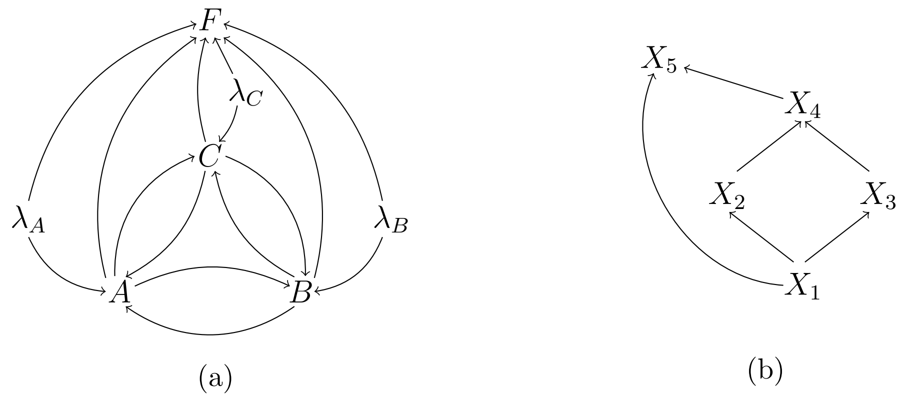


Figure 2.1: Examples: (a) shows a directed graph with directed cycles; (b) shows a DAG.

As is common and convenient, terms of kinship will be used to refer to relations between vertices in a directed graph G: given a vertex X its set of parents, denoted $Pa(X)$, contains all those vertices with an arrow to X and its set of children, denoted $Ch(X)$, contains all those vertices to which there is an arrow from X. Similarly, an ancestor of X is a vertex with a directed path to X and a descendant of X is a vertex to which there is a directed path from X.

Chapter 6 will also make use of *hypergraphs*, which are a generalisation of undirected graphs. A hypergraph is given by a set V of vertices and a set of hyperedges, each of which is undirected and may generally connect more (or fewer) than two vertices. The set of hyperedges is formally given by a subset of the powerset of V. Examples will be given in Chapter 6.

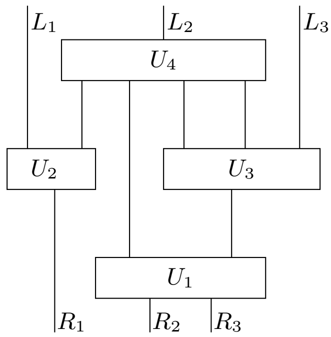


Figure 2.2: Example of a circuit diagram.

Finally, *circuit diagrams* will be a convenient way of representing compositional structure between quantum systems and the maps between them. See Fig. 2.2 for an example. The convention in this thesis is to read them bottom up.

An introduction into a formal and fully diagrammatical representation of quantum theory can be found in the textbook in Ref. [91]. Roughly speaking, in a circuit diagram wires represent systems, boxes represent linear maps, parallel composition in the diagram corresponds to tensor product composition and connecting up boxes with wires corresponds to the composition of the corresponding linear maps. In this way a circuit diagram may represent two distinct kinds of data: either linear maps between the Hilbert spaces associated with quantum systems (at that level only unitary maps will be represented in circuit diagrams in this thesis), or CP maps, i.e. linear maps at the level of spaces of operator on the underlying Hilbert spaces. The context will always make clear which kind of data a diagram represents. In case a diagram represents CP maps an upside-down grounding symbol represents the CPTP map defined by the partial trace.

Chapter 3

Background

3.1 Classical causal models

3.1.1 Introduction and definition

The framework of classical causal models, initially developed by Spirtes *et al.* [8] and Pearl [9], addresses and formalises causal reasoning about classical random variables. As mentioned in Chapter 1, it does so by spelling out, in a rigorous manner, what the relation is between the assertion of causal relations between variables and statistical statements about them. The past 40 years have seen the development of a vast body of literature on causal models, but the following summary, which in many respects will follow the presentation by Pearl in Ref. [9], will not attempt to do justice to the history or breadth of that field, but instead will focus on the conceptual and technical skeleton, so as to provide the basis for the subsequent study of 'quantum causal reasoning'.

Given a finite set of random variables[1] $X_1, \ldots, X_n$, its causal structure is represented by a DAG with vertices $X_1, \ldots, X_n$ such that an arrow $X_i \to X_j$ stands for that X_i is a *direct cause* of X_j[2]. Using terms of kinship (see Sec. 2.3), any ancestor of X_j, which is not a parent, also is a cause of X_j, albeit an indirect one, the idea being that the causal influence is mediated via the intermediate causes[3].

A causal model specifies the relationship between the causal structure of variables $X_1, \ldots, X_n$ as expressed by a DAG and a probability distribution over $X_1, \ldots, X_n$ as follows.

[1]Recall from Sec. 2.1 that random variables are assumed throughout to take values in sets of finite cardinality.

[2]Directed graphs with directed cycles are sometimes used to represent feedback loops, however, will not be considered in the present exposition. Also see the discussion in Sec. 7.6.

[3]The distinction between direct and indirect causes thus manifestly depends on the choice of variables. Also see Sec. 8.3.

Definition 3.1 (Classical causal model): *A classical causal model (CCM) is given by*

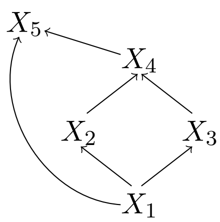
(1) *a causal structure represented by a DAG G with vertices corresponding to random variables* $X_1, \ldots, X_n$*,*

(2) *for each* X_i*, a classical channel* $P(X_i|Pa(X_i))$*.*

The classical causal model defines a probability distribution over $X_1, \ldots, X_n$*, given by*

$$P(X_1, ..., X_n) = \prod_i P(X_i|Pa(X_i)). \tag{3.1}$$

See Fig. 3.1 for a generic example of a classical causal model.



$$P(X_1, X_2, X_3, X_4, X_5) = P(X_5|X_1, X_4)\ P(X_4|X_2, X_3)\ P(X_2|X_1)\ P(X_3|X_1)\ P(X_1)$$

Figure 3.1: A classical causal model.

Insofar as a causal model plays the role of a causal explanation, the idea is that a probability distribution $P(X_1, ..., X_n)$, which might in particular be obtained from actual observational data, is the explanandum and can be explained causally in terms of the DAG G if it admits a causal model that involves G such that Eq. (3.1) holds — the explanans thus consisting in G and the set of channels $P(X_i|Pa(X_i))$. It is therefore convenient to capture the corresponding property of a probability distribution relative to a DAG as follows.

Definition 3.2 (Markov condition): *Given a DAG G, with vertices corresponding to random variables* $X_1, \ldots, X_n$*, a joint probability distribution* $P(X_1, \ldots, X_n)$ *is called* Markov *for G if and only if there exist classical channels* $P(X_i|Pa(X_i))$ *such that*

$$P(X_1, \ldots, X_n) = \prod_{i=1}^{n} P\big(X_i|Pa(X_i)\big)\ . \tag{3.2}$$

The data of a causal model can then be stated as a pair $(G, P(X_1, \ldots, X_n))$, where G is a DAG with vertices $X_1, \ldots, X_n$ and $P(X_1, \ldots, X_n)$ a probability distribution that is Markov for G[4].

Given only a probability distribution $P(X, Y, Z)$ one can — provided that it is well-defined — calculate Bayesian conditionals, say $P(Y|X)$, and on that basis make predictions for the probability of observing $Y = y$ given that one has observed $X = x$. A very different scenario is one in which an agent intervenes on variable X and forces it to take on the value x. Such 'reaching in' from external to the situation described by $P(X, Y, Z)$ changes the causal structure of the variables X, Y, Z. The original distribution $P(X, Y, Z)$ as such thus has nothing to say about the new situation.

However, suppose instead a causal model is given that explains $P(X, Y, Z)$ that involves some DAG G with vertices X, Y, Z. The idea is that the causal relations expressed in G stand for causal mechanisms between the variables and an important assumption for classical causal models is that these mechanisms are stable and autonomous. Hence, knowing G and the effective description of the causal mechanisms through the channels $P(X_i|Pa(X_i))$, should allow one to specify which new causal situation arises upon an intervention. This is very much akin to a 'mechanic's understanding of a machine', on the basis of which one can replace parts while leaving others, that is, in particular their function, unaltered and build a new whole. A particularly important intervention is a do-intervention $do(X = x)$, which is the intervention on X described above that forces X to take the value x, thereby overriding the causal mechanism which would have fixed X otherwise in the pre-intervention scenario. More generally, consider a do-intervention on a set S of variables, denoted $do(S = s)$, meaning that each variable X in S is forced to take the value x as given by the tuple s. The following spells out how a causal model allows going from a pre- to a post-do-intervention distribution.

Definition 3.3 (Do-conditional distribution): *Consider a classical causal model given by a DAG G with nodes $X_1, \ldots, X_n$, and for each i a classical channel $P(X_i|Pa(X_i))$. Let $S \subset \{X_1, ..., X_n\}$ and let $T := \{X_1, ..., X_n\} \setminus S$. The* do-conditional distribution *for T, given a do-intervention on S, is given by*

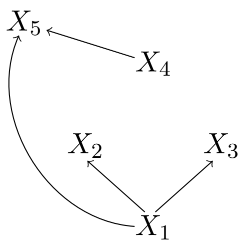
$$P(T|do(S)) := \prod_{X_i \in T} P(X_i|Pa(X_i)). \tag{3.3}$$

[4] In the literature this Markov condition (or equivalent formulations) is sometimes referred to as the 'causal Markov condition' [8,92], emphasising that the DAG is given a causal interpretation. Also note that in our presentation the Markov condition is stated in terms of asserted channels, rather than conditional distributions obtained from the given joint probability distribution — the given probability distribution may not have full support but still admit of a causal model.

If s is a particular value of S, i.e., a tuple containing a value for each variable $X_i \in S$, then

$$P(T|do(S=s)) := \left(\prod_{X_i \in T} P(X_i|Pa(X_i)) \right) \Bigg|_{S=s} . \tag{3.4}$$

Given a do-conditional distribution $P(T|do(S))$, marginals are calculated as usual, i.e. $P(X_i|do(S)) := \sum_{X_j \in T, j \neq i} P(T|do(S))$, seeing as $P(T|do(S))$ just is an ordinary probability distribution over T (for every value $S = s$), where $do(S)$ is a mere reminder of how it arises. For obvious reasons, Eq. 3.3 is also referred to as the *truncated factorization formula*, since it effectively throws away all factors in the product of Eq. 3.2 that correspond to variables that are being do-intervened on. See Fig. 3.2 for an example.



$$P(X_1, X_2, X_3, X_5|do(X_4 = x)) = P(X_5|X_1, X_4 = x) \; P(X_2|X_1) \; P(X_3|X_1) \; P(X_1)$$

Figure 3.2: Example: a do-intervention on X_4 is performed. Suppose the causal structure prior to that was as in Fig. 3.1, then $do(X_4 = x)$ overrides the mechanism from the parents of X_4, in this case, X_2 and X_3, which is reflected in the mutilated DAG shown above, in which the arrows into X_4 have been removed. The new causal structure explains the properties of $P(X_1, X_2, X_3, X_5|do(X_4 = x))$.

Note that prior to the advent of causal models, Bayesian networks had been studied, which can also be defined as a DAG, together with a distribution that is Markov for it[5] [9, 93]. A given probability distribution $P(X_1, \ldots, X_n)$ is Markov for many different DAGs (also see Sec. 3.1.3), however, only if a DAG G represents the causal structure, the do-conditional distributions according to Def. 3.3 will make actually correct predictions — something that can in principle be verified experimentally.

3.1.2 Causal principles — why the Markov condition?

At this point the main question that arises is, why these causal models should correctly guide causal reasoning. Why that Markov condition? There are of course deep questions concerning the (metaphysical) status of causal relations, such as

[5] Note that in this case the Markov condition is in terms of the conditional distributions obtained from the given joint distribution and not in terms of separate classical channels. This makes only a difference where the distribution does not have full support, see footnote [4].

whether they can be further reduced to, and thereby grounded in, probabilistic, interventional, counterfactual, or other relations. What is the relation to the arrow of time? Such questions are still being debated in philosophy (see, e.g., Refs. [92,94]) and answers will depend on one's preferred philosophical programme. Even though ultimately such questions cannot be ignored in asking about the status of causal models, in light of their empirical success and relevance, it seems fair to ask at least, suppose there are causal relations — whatever their status is — why would they relate to statistical claims as the causal models have it. After all, the framework is to be used in serious decisions in, e.g., medicine or economics.

Reichenbach's common cause principle [5] can be seen to be at the heart of causal models and raise similar questions. Due to its historical importance in the role it played in understanding the link between causal and probabilistic claims, and for later reference, it is worth paraphrasing it again here in slightly more detail than in the introduction: Given two variables Y and Z and a probability distribution $P(Y, Z)$, if they are statistically correlated, i.e. $P(Y, Z) > P(Y)P(Z)$, then there ought to be a causal explanation of that fact in terms of either Y being a cause of Z, Z being a cause of Y, that there is a common cause X, or else a combination of the latter with one of the former two. In case neither of Y and Z is a cause of each other and X is a *complete common cause*, that is, no further common causes are missing, then Y is statistically independent from Z conditional on X, i.e. $P(Y, Z|X) = P(Y|X)P(Z|X)$ (also see Sec. 3.1.3).

Observing that the condition $P(Y, Z|X) = P(Y|X)P(Z|X)$ is equivalent to that for the joint distribution over all three variables it holds that $P(Y, Z, X) = P(Y|X)P(Z|X)P(X)$, the common cause principle can be seen as a special case of the following causal principle, which is in keeping with the definition of a causal model.

Principle 1 (General causal principle): *Given variables $X_1, \ldots, X_n$, if their causal structure is as in the DAG G with vertices $X_1, \ldots, X_n$, with no common causes missing, then the probability distribution describing $X_1, \ldots, X_n$ is Markov for G.*

The question of this section can thus be phrased as, on what grounds can Principle 1 be justified? Why should the Markov condition be a reasonable constraint on a probability distribution from causal structure — a question that stands quite independently from one's preferred interpretation of probabilities. Some advocate a normative status of the principle in that it guides us in finding an appropriate set of variables for causal reasoning (see, e.g., Refs. [8, 92]). In contrast, Pearl offers a different perspective in Ref. [9], which will be sketched here (following Ref. [4] in its presentation). This is not to be taken as a binding suggestion, but as a pedagogical analysis that will be particularly instructive for the analysis in the quantum case.

In this view, causal relations between variables $X_1, \ldots, X_n$ as represented by a DAG G are taken to stand for functional dependences in an underlying functional model as defined in Ref. [9]. If X_i has parents $Pa(X_i)$ in G, then it functionally depends on the variables in $Pa(X_i)$ through the function f_i that determines the variable X_i. The way probabilities enter the stage from such a deterministic level of description is that there are typically further causes not included in $X_1, \ldots, X_n$, which can either not be accessed or, one does not care about, so that the lack of knowledge over their values cannot but be encoded in a probability distribution. Now for G to be the causal structure of $X_1, \ldots, X_n$ without missing common causes means that the additional causes are at most 'local disturbances', i.e. for each X_i there may be an additional variable λ_i such that λ_i is at most a cause of X_i. A functional model involving the DAG G as causal structure specifies functions of the form $f_i : Pa(X_i) \times \lambda_i \to X_i$ that determine each variable via $X_i = f_i(Pa(X_i), \lambda_i)$, together with a product distribution $P(\lambda_1, \ldots, \lambda_n) = \prod_i P(\lambda_i)$, assuming the local disturbances to be statistically independent. The probability distributions over $X_1, \ldots, X_n$ that arise from marginalising over the local disturbances λ_i are those distributions that can be causally explained by G. More formally,

Definition 3.4 (Compatibility with a DAG): *Given a DAG G with vertices $X_1, \ldots,$ X_n, a joint probability distribution $P(X_1, \ldots, X_n)$ is* compatible *with G if and only if there exist n additional variables $\lambda_1, ..., \lambda_n$ and functions $f_i : Pa(X_i) \times \lambda_i \to X_i$, along with distributions $P(\lambda_i)$ such that*

$$P(X_1, \ldots, X_n) = \sum_{\lambda_1, \ldots, \lambda_n} \left[\prod_{i=1}^{n} \delta\Big(X_i, \; f_i(Pa(X_i), \lambda_i) \Big) \; P(\lambda_i) \right] . \tag{3.5}$$

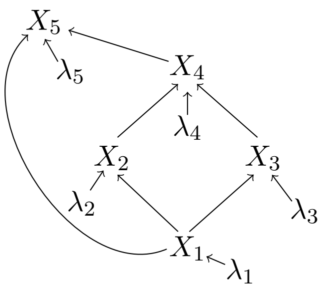
The assumption that the local disturbances can be ascribed a product distribution is a substantial, but common assumption, which will not be further justified here (also see an analogous discussion in Sec. 5.2.4). Importantly, the following equivalence holds.

Theorem 3.1 (Equivalence of classical compatibility and Markovianity [9]): *Given a distribution $P(X_1, \ldots, X_n)$ and a DAG G with vertices $X_1, \ldots, X_n$, the following are equivalent:*

(1) *$P(X_1, \ldots, X_n)$ is compatible with G.*

(2) *$P(X_1, \ldots, X_n)$ is Markov for G.*

If defining causal relations as functional relationships between variables given underlying deterministic evolution, and if assuming that local disturbances can be treated as statistically independent, then it is those probability distributions $P(X_1, \ldots, X_n)$ that are compatible with a DAG G that can be causally explained by G. Thm. 3.1 establishes that this set is the same as those that are Markov for G. The theorem can therefore be seen to justify Principle 1 and the definition of a classical causal model — on the basis of the assumptions.



$$
\begin{aligned}
X_5 &= f_5(X_1, X_4, \lambda_5), \\
X_4 &= f_4(X_2, X_3, \lambda_4), \\
X_3 &= f_3(X_1, \lambda_3), \\
X_2 &= f_2(X_1, \lambda_2), \\
X_1 &= f_1(\lambda_1), \\
P(\lambda_1, \lambda_2, \lambda_3, \lambda_4, \lambda_5) &= \prod_{i=1}^{5} P(\lambda_i)
\end{aligned}
$$

.

Figure 3.3: A functional model as it can be seen to underly the causal model in Fig. 3.1.

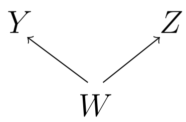
This view of causal relations as functional dependences also allows to understand the truncated factorisation formula from Eq. (3.4) for calculating do-conditional distributions. Let a functional model for variables $X_1, \ldots, X_n$ be given by the family of functions $f_i : Pa(X_i) \times \lambda_i \to X_i$ and distributions $P(\lambda_i)$. Let $S \subset \{X_1, \ldots, X_n\}$ and $T := \{X_1, \ldots, X_n\} \setminus S$. A do-intervention $do(S = s)$ corresponds to (1) deleting all equations $X_i = f_i(Pa(X_i), \lambda_i)$ for $X_i \in S$, since the corresponding mechanisms are overridden by $do(S = s)$, and (2) wherever $X_i \in S$ appears as a parent of a variable in T, fixing the value of X_i according to $S = s$. It is straightforward to see that at the probabilistic level, once marginalised over the local disturbances λ_i of the variables in T, then the right-hand side of Eq. (3.4) is obtained as the correct expression for the post-do-intervention probability distribution for the remaining variables.

3.1.3 Conditional independence and the d-separation theorem

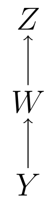
Given a probability distribution $P(Y, Z, W)$, the (sets of) variables Y and Z are statistically independent conditional on (set) W, written $(Y \perp\!\!\!\perp Z|W)_P$, if and only if $P(Y, Z|W = w) = P(Y|W = w)P(Z|W = w)$ whenever $P(W = w) \neq 0$.

Statistical (unconditional) independence between Y and Z is the special case of $W = \emptyset$ and hence denoted $(Y \perp\!\!\!\perp Z)_P$.

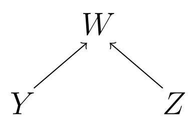
Consider the situation from Sec. 3.1.2 that Reichenbach's common cause principle is concerned with. There, the fact about a given probability distribution $P(Y, Z, W)$ in need of explanation is the correlation between, say Y and Z, i.e. that $(Y \not\!\perp\!\!\!\perp Z)_P$. Suppose the causal structure is as in Fig. 3.4a, featuring W as a complete common cause. The sense in which this achieves a successful explanation as demanded by the principle is that then $(Y \perp\!\!\!\perp Z|W)_P$ holds, which is in particular true if $P(Y, Z, W)$ is Markov for the fork in Fig. 3.4a. The idea is that the correlation disappears once one conditions on the value of the common cause W, because the variable W that underwrote the correlation in the first place, is held fixed.



(a) A fork.



(b) A chain.



(c) A collider.

Figure 3.4

Similarly, suppose $P(Y, Z, W)$ is given and $(Y \not\!\perp\!\!\!\perp Z)_P$ holds, but the causal structure is as in Fig. 3.4b. That Y and Z are correlated is again expected seeing as the former is a cause of the latter, however this is not a direct cause relation, but an indirect one via W. The Markov condition for the chain in Fig. 3.4b demands that $P(Y, Z, W) = P(Z|W)P(W|Y)P(Y)$. Again, this implies that $(Y \perp\!\!\!\perp Z|W)_P$ — the correlation between Y and Z is explained through its disappearance upon conditioning on the variable W that mediates the 'creation of the correlation'. In contrast, if the causal structure is as in Fig. 3.4c (not assuming $(Y \not\!\perp\!\!\!\perp Z)_P$), the Markov condition demands that $P(Y, Z, W) = P(W|YZ)P(Y)P(Z)$. Then Y and Z are statistically independent as one would expect since they are causally unrelated. However, conditioning on the collider W will typically render them correlated, i.e. one finds $(Y \not\!\perp\!\!\!\perp Z|W)_P$. Such a case is thus clearly distinguished from the first two cases of the fork and chain.

Conditional and unconditional independence relations as well as their absences are thus at the heart of giving (classical) causal explanations. In the canonical examples of the fork, chain and collider above, the Markov condition did exactly what one expected. This leads to the more general question concerning what the relation between conditional independence relations in a distribution P and a causal structure G is, provided P is Markov for G so that the latter can be regarded the causal structure in keeping with Principle 1.

The graphical criterion that has been found to capture which conditional independence relations hold in a distribution that is Markov for a DAG, is called *d-separation*. The precise definition below is a little lengthy at first sight, but becomes intuitive with the three canonical examples form above in mind — in Figs. 3.4a and 3.4b Y is d-separated from Z by W, in contrast to Fig. 3.4c.

Definition 3.5 (Blocked paths and d-separation [95]): *Given a DAG G, a path between vertices y and z is* blocked *by the set of vertices W if the path contains either*

(1) *a chain $a \to w \to c$ or a fork $a \leftarrow w \to c$ with the middle vertex $w \in W$*

(2) *a collider $a \to r \leftarrow c$ such that neither r nor any descendant of r lies in W.*

For subsets of vertices Y, Z and W, say that Y and Z are d-separated *by W, and write $(Y \perp\!\!\!\perp Z|W)_G$, if for every $y \in Y$ and $z \in Z$, every path between y and z is blocked by W.*

A fundamental theorem of the framework then is the following.

Theorem 3.2 (d-separation theorem [96, 97], also see Ref. [9]): *Consider a DAG G, with vertices $X_1, \ldots, X_n$, and disjoint subsets of vertices Y, Z, and W.*

(1) *(Soundness): if $(Y \perp\!\!\!\perp Z|W)_G$, then any distribution $P(X_1, \ldots, X_n)$ that is Markov for G satisfies $(Y \perp\!\!\!\perp Z|W)_P$.*

(2) *(Completeness): if $(Y \not\perp\!\!\!\perp Z|W)_G$, then there exists a probability distribution $P(X_1, \ldots, X_n)$ such that $P(X_1, \ldots, X_n)$ is Markov for G and $(Y \not\perp\!\!\!\perp Z|W)_P$.*

Note that the d-separation theorem does not rely on a causal reading of the DAG and equally holds in the context of Bayesian networks. What the examples in Fig. 3.4 made plausible is that if they do express the respective causal structure then one would indeed also expect the conditional independence relations to hold that are implied by Markovianity. However, a probability distribution $P(X_1, \ldots, X_n)$ is Markov for many different DAGs[6]. This fact in turn makes Thm. 3.2 highly relevant to causal discovery.

[6]Observe that, given a probability distribution $P(X_1, \ldots, X_n)$, for every possible total order of the variables $X_1, \ldots, X_n$, it is immediate from the chain rule for probability distributions that $P(X_1, \ldots, X_n)$ is Markov for the 'completely connected' DAG corresponding to that total order of $X_1, \ldots, X_n$.

Suppose a probability distribution $P(X_1, \ldots, X_n)$ is given that is estimated from observational data. The *problem of causal discovery* is finding what a plausible causal explanation is, that is, finding which additional assumptions are needed so that the causal structure could be, as far as possible, singled out in a principled and convincing way.

By putting the causal principle (Principle 1) to work one can exclude any DAG with vertices $X_1, \ldots, X_n$, for which $P(X_1, \ldots, X_n)$ is not Markov. Under the assumption that there are no latent common causes, i.e. there are no common causes that are not already included in $X_1, \ldots, X_n$, at first instance the problem becomes classifying all DAGs with vertices $X_1, \ldots, X_n$, for which a distribution is Markov. This is why the d-separation theorem can easily be understood to be at the heart of the celebrated causal discovery algorithms [96,98]. A common further assumption is that the correct causal explanation is given by a *faithful causal model.* Faithfulness requires that $P(X_1, \ldots, X_n)$ does not satisfy any further 'extraneous' conditional independence relations that are not enforced by a corresponding d-separation relation in the DAG. This is a plausible desideratum for a good explanation because 'extraneous' conditional independences would require careful *fine-tuning* of the parameters of a functional causal model. One is then looking for exactly the DAGs G that have those and only those d-separation relations $(Y \perp\!\!\!\perp Z|W)_G$ that have a corresponding conditional independence relation $(Y \perp\!\!\!\perp Z|W)_P$ in the distribution P. Finding these in a systematic way is what the causal discovery algorithms achieve and output. Further assumptions such as the time ordering of variables may then be invoked, if such knowledge is available, to reduce the set of DAGs[7].

In case no assumption is made with regards to whether or not there are latent common causes, the situation is more difficult. However, algorithms have been developed that output sets of DAGs, involving possible further latent variables, that are the candidate causal explanations given plausible assumptions [8,9]. While these causal discovery algorithms are among the strongest achievements of the framework, they will not be presented in more detail, as they are not needed for the remainder of the thesis.

[7]For instance, given $P(Y, Z, W)$, note that $(Y \perp\!\!\!\perp Z|W)_P$ is equivalent to Markovianity for the fork in Fig. 3.4a, but also to Markovianity for the chain in Fig. 3.4b. These two causal structures are thus not distinguishable just given $P(Y, Z, W)$, without further assumptions, e.g. about the time ordering of the variables. (Note that both, the fork and chain, would constitute faithful causal models if $(Y \perp\!\!\!\perp Z|W)_P$ holds, hence, faithfulness does not distinguish them either.)

3.1.4 The do-calculus

Being able to assess the causal effect of X on Y, which is how Pearl also refers to the do-conditional probability $P(Y|do(X))$ [9], is obviously of great relevance to many fields, be it medicine or economics. Knowing $P(Y|do(X))$ is about both, finding out whether Y wiggles at all as X wiggles, but also how much so. If one can conduct an experiment in which one controls X, that is, intervenes on X, then $P(Y|do(X))$ can be determined experimentally. There are however cases where such an intervention is practically impossible or considered unethical. Of the latter kind is the famous example that one cannot force a control group of humans to smoke so as to find out how strong the causal effect of smoking on lung cancer is. This would however be necessary to assess the plausibility of the genotype theory, defended by the tobacco industry at some point, which proposed to explain the correlation between smoking and lung cancer through a confounding common cause of a genetic nature that increases the craving for nicotine and the probability to suffer from lung cancer.

The preceding introduction of causal models established two things. First, just given a probability distribution $P(X, Y, ...)$, the causal effect $P(Y|do(X))$ can in principle not be calculated. It has to be supplemented with causal knowledge. Second, if a causal model for $P(X, Y, ...)$ with causal structure G is given, then it is easy to calculate $P(Y|do(X))$ through employing the truncated factorisation formula from Eq. (3.3). However, what if the whole distribution over all causally relevant variables that appear in G is *not* known? Suppose a DAG G correctly represents the actual causal structure — maybe the judgment of some expert or in combination with the output of a causal discovery algorithm — but only some of the variables in G are observed. When and how can one then calculate the causal effect $P(Y|do(X))$? This is the problem of the identifiability of causal effects [9].

The framework of causal models solves this problem as well as is in principle possible, through the so called *do-calculus* [9], one of the framework's main achievements. This do-calculus comprises a set of three inference rules that relate observational and interventional statements — warranted by certain properties of the causal structure G. It does so in a way that helps to express the desired causal effect $P(Y|do(X))$ entirely in terms of objects computable from the given distribution and G, typically through multiple application of the rules. Crucially, these three rules were proven to be complete for the problem of causal effect identifiability [9], that is, a causal effect is computable if and only if it can be obtained through a finite sequence of applications of the three rules.

The below theorem states the three rules, each of which is of the form that a graphical antecedent in terms of a mutilated version of G implies an equality that relates a Bayesian and a do-conditional probability distribution. The notation follows the one from Ref. [9], in particular, given a DAG G, if S is a subset of its vertices, then $G_{\overline{S}}$ denotes the DAG that is obtained from G by removing all arrows incident on vertices in S and conversely, $G_{\underline{S}}$ denotes the DAG, where all arrows have been removed from G that are going out of vertices in S.

Theorem 3.3 (Rules of the do-calculus for classical causal models [9]): *Let a classical causal model be given by a DAG G and a probability distribution $P(...)$*[8]*. Let X, Y, Z, and W be disjoint subsets of the variables.*

Rule 1 *(insertion/deletion of observations):*

$$(Y \perp\!\!\!\perp Z | X, W)_{G_{\overline{X}}} \quad \Rightarrow \quad P(Y|do(X), Z, W) = P(Y|do(X), W)$$

Rule 2 *(exchange of observations and interventions):*

$$(Y \perp\!\!\!\perp Z | X, W)_{G_{\overline{X}\underline{Z}}} \quad \Rightarrow \quad P(Y|do(X), do(Z), W) = P(Y|do(X), Z, W)$$

Rule 3 *(insertion/deletion of interventions):*

$$(Y \perp\!\!\!\perp Z | X, W)_{G_{\overline{X},\overline{Z(W)}}} \quad \Rightarrow \quad P(Y|do(X), do(Z), W) = P(Y|do(X), W) \ ,$$

where $Z(W)$ denotes the set of nodes in Z that are not ancestors of W in $G_{\overline{X}}$.

Note that Rule 1 contains the soundness part of the d-separation theorem, Thm. 3.2, as the special case given by $X = \emptyset$. As the focus in this thesis does not lie on the application of these rules to identify causal effects, the presentation contents itself with giving the basic idea as done above. Further intuition for each rule will be built when studying the quantum analogues in Sec. 5.6.

3.2 The path to quantum causal models

3.2.1 Why quantum causal models?

The framework of classical causal models, summarised in the previous section, fails to provide the grounds to give satisfactory causal explanations of the correlations one does encounter in experimental data when quantum systems are involved. Let us recapitulate the standard argument, already mentioned in Chapter 1, for why that is the case by appealing to Bell's theorem [11, 12].

[8] As with conditional independence relations, wherever conditional probabilities appear in the consequents of the three rules this is to be understood as that the equality holds for all values of the variables for which the conditional distribution is defined.

Suppose then that at a region A a pair of two-dimensional systems, A_1 and A_2, say two photons, are prepared in a Bell state, say $(1/\sqrt{2})(|00\rangle + |11\rangle)$. They are then sent off to space-like separated regions B and C, where agents are stationed and both parties perform one out of two possible, appropriately chosen measurements, say spin S_X or S_Z. Let the outcomes at B and C be denoted k_B and k_C, respectively, and their choices of measurements τ_B and τ_C, respectively. Upon comparing measurement statistics one will find the outcomes are correlated in the conditional distribution for fixed measurements, i.e. $P(k_B, k_C|\tau_B, \tau_C) \neq P(k_B|\tau_B)P(k_C|\tau_C)$, where it was used that $P(k_B|\tau_B, \tau_C)$ does not depend on τ_C and, similarly, $P(k_C|\tau_B, \tau_C)$ not on τ_B, in keeping with relativity given that the regions are space-like separated. For the same reason k_B and k_C cannot be causes of each other. Reichenbach's common cause principle then demands that there ought to exist a common cause λ in the past such that $P(k_B, k_C|\tau_B, \tau_C, \lambda) = P(k_B|\tau_B, \lambda)P(k_C|\tau_C, \lambda)$. However, Bell's theorem essentially states that from the previous expression an inequality can be derived, which quantum theory predicts to be violated, e.g., for the outlined scenario where a Bell state is prepared.

The fact that Bell-inequality violations have been confirmed in numerous experiments is therefore typically taken to imply a failure of Reichenbach's common cause principle — there can in principle not exist a variable in the common past of B and C that would warrant a common cause explanation as the principle demands. The principle however essentially *is* what a common cause explanation within classical causal modeling would amount to and thus is a general pillar of classical causal models (see Sec. 3.1.2). The existence of Bell inequality violating correlations via Bell's theorem only implies the invalidity of the conjunction of all assumptions that go into the theorem (which have not been made explicit here), and it is well-known that there are ways to retain an explanation of Bell correlations in terms of classical variables. These explanatory strategies, such as invoking superdeterminism, retro-causal influences or superluminal causal influences, can be treated as giving causal explanations within the framework of classical causal models, however, as Wood and Spekkens showed in Ref. [13], and further elaborated by Cavalcanti in Ref. [99], necessarily at the cost of relying on some form of fine-tuning (see Sec. 3.1.3). If a common and fundamental phenomenon of quantum systems such as Bell-nonlocal correlations *always* requires fine-tuning, then this may well be taken to mean that it cannot be explained causally with classical causal models.

While quantum correlations go beyond what is explicable in terms of classical causal models, in a sense, there is nothing puzzling about the Bell scenario as far as giving a causal account of it from within the quantum formalism is concerned — the intuition is that there is an obvious common cause: the preparation of a Bell state at A. And this is of course the whole point here; it seems as if there may not be an in principle obstacle to giving causal explanations once one allows quantum systems to take the role of causal relata in some form or other, and provided one adjusts what a successful causal explanation is taken to mean, i.e. not the factorisation property in a classical conditional probability distribution. Such hope was formulated and argued for by Wood and Spekkens in Ref. [13] (also see the work by Cavalcanti and Lal in Ref. [100]). What this calls for is a quantum framework that makes the intuition of 'quantum causal explanations' rigorous.

There is a large body of literature with a series of strong results due to Rédei, Hofer-Szabó and their collaborators (see, e.g., Refs. [101–108]), exploring, in particular, whether a (generalised) common cause principle can be maintained in light of quantum theory. The intention of this research programme and the underlying notion of a (generalised) common cause explanation are somewhat complementary to those in this thesis (see, e.g., Refs. [78, 100] for discussions).

3.2.2 Previous approaches I

The past couple of decades have seen much work dedicated to the development of a quantum generalisation of causal models. It is not possible to cover all of it here and to do full justice to the different kinds of ideas that have appeared or to the different aspects with respect to which one could delineate them. Good overviews, that the following one is inspired by, can be found in Refs. [4,82]. The works that are going to be mentioned all share the usage of DAGs and that they involve quantum systems in some way or other. The main themes are: What data does the DAG represent? What do the arrows mean? What object is constrained by the DAG? Can one treat arbitrary interventions on a set of quantum systems? In what sense does it allow to give causal explanations? It may be helpful to identify five broad groups of works prior to and distinct from the approach taken in this thesis, which is the sixth group, as it were, that was begun in the work by Allen *et al.* in Ref. [4] to be summarised in detail in Sec. 3.2.5. Concerning the first five groups it may further be helpful to distinguish those that rely on the quantum process formalism and those that do not. Hence, the overview is split accordingly into two parts — Secs. 3.2.2 and 3.2.4 — to give way to the 'intermezzo' that introduces the process formalism.

First, the earliest works noteworthy in this context, which add quantum systems to the data represented by a DAG are those by Tucci in Refs. [73, 74]. It associates complex probability amplitudes with the vertices of the DAG, in order to achieve what might be seen as a quantum analogue of Bayesian networks, that is, it does not insist on a causal interpretation of the DAG.

Second, there is a group of works, including those in Refs. [34, 35, 77, 80, 81], that do not all have identical goals, but share the features that (1) the DAG is intended to have a causal reading and involves quantum systems and (2) the object constrained by a causal DAG is a probability distribution over classical variables that represent the settings and outcomes of measurement of the quantum systems. A 'causal arrow' is here taken to represent the passing of quantum systems between the loci, where the measurements take place, which are in turn represented by the vertices. Generally, these works are concerned with how the bringing in of quantum resources changes the interplay between causal structure, on the one hand, and equality and inequality constraints on the associated probability distribution, on the other hand.

More specifically, the works by Henson, Lal and Pusey in Ref. [34] and by Fritz in Ref. [35] develop a set-up in order to derive generalised Bell inequalities in arbitrary causal scenarios (also see, e.g., Refs. [13, 36–38]). Both, Ref. [34] and also the work by Pienaar and Brukner in Ref. [80] study the ramifications of d-separation in the presence of quantum systems and achieve the derivation of generalisations of the classical d-separation theorem (see Sec. 3.1.3). However, due to the fact that the object constrained by causal structure maintains to be a classical distribution, it is not a fully quantum version of the theorem and cannot capture whether or not, loosely speaking, 'd-separation between quantum systems' captures a genuine notion of quantum conditional independence.

Related to this second group, in so far as a quantum causal model specifies a probability distribution over classical variables that is constrained by a causal DAG, is the recent approach developed by Pienaar in Refs. [85–88]. Otherwise, it however is quite distinct from the above mentioned approaches and can be seen as the application of the QBist take on quantum theory [109] to causal modeling. The probability distribution, specified by a quantum causal model, arises specifically from considering symmetric informationally-complete positive operator-valued measurements on the quantum systems. A special feature of these quantum causal models is that the proposed quantum Markov condition is preserved under the reversal of all arrows in the DAG.

A third group of works is situated in the context of aiming at a formulation of the quantum formalism as a theory of Bayesian inference as undertaken in Refs. [75, 76, 78]. The work by Leifer and Poulin in Ref. [76] presented approaches to quantum generalisations of various ways in which DAGs have been employed in classical probability theory. In particular Ref. [76] proposed a notion of 'quantum Bayesian networks' (therein called quantum Markov networks), where a DAG has vertices that represent Hilbert spaces and the constraints it imposes on a quantum state over all involved Hilbert spaces are in terms of quantum conditional mutual information. Ref. [76] inspired much later work, including this thesis. In Ref. [78] Leifer and Spekkens further developed the ideas and used a particular definition of quantum states and quantum conditional states as proposed analogues to classical joint and conditional probability distributions so as to provide a similarly causally-neutral way for inference about quantum systems, i.e. that can be used to formalise reasoning about quantum systems regardless of the causal relations amongst them. They then studied how different causal scenarios constrain a quantum (conditional) state, working towards a corresponding quantum approach to causal models. In contrast to the previous approaches, here the object constrained by a DAG is not a classical probability distribution, but an intrinsically quantum object. There are however serious obstacles to a fully general treatment based on associating single Hilbert spaces with the vertices of the DAG [110]. Also note that while the DAG is intended to encode causal relations, there is no precise definition of causal relations between quantum systems.

Recall that a classical causal model allows to make predictions for post-intervention scenarios[9]. This additional power, brought about by giving the DAG a causal interpretation as done in a causal model, can be considered *the* decisive difference to Bayesian networks. Now, note that a similar 'predictiveness for arbitrary quantum interventions' is a feature that all of the above mentioned approaches to quantum generalisations of causal models lack[10]. While the probability distribution, constrained by causal structure in the second group above, is taken to arise from the quantum systems through a measurement process, it is not the case that the data that *defines the model* allows to calculate outcome probabilities for arbitrary interventions on the quantum systems.

Other approaches to quantum generalisations of causal models have in contrast focused on that aspect. Although it need not be that way, many of them happen to also stand in a tradition of taking an operationalist perspective on quantum theory, together with an interventionist account of causation.

Intuitively speaking, the core behind an interventionist account of causation is the idea that what it means to say that C is a cause of E is that, when an agent

[9]Although often only do-interventions are considered, in principle arbitrary interventions could be treated (see Sec. 5.3).

[10]The mentioned work by Pienaar does allow to consider arbitrary interventions, however, only for special cases of DAGs (see Refs. [86, 88]).

'wiggles on C', then also 'E wiggles', that is, through manipulating C one can send signals to E[11]. Classically, this is conveniently formalised as follows. Given a classical channel $P(EF|CD)$, variable C can signal to E, if and only if for at least some value d it holds for the marginal channel that $P(E|C=c, D=d) \neq P(E|C=c', D=d)$ for some $c \neq c'$.

Similarly, given a quantum channel $\mathcal{E} : \mathcal{L}(\mathcal{H}_C \otimes \mathcal{H}_D) \to \mathcal{L}(\mathcal{H}_E \otimes \mathcal{H}_F)$, system C is said to be able to signal to E if and only if for at least some state ρ_D it holds that the marginal states differ for some $\rho_C \neq \rho'_C$, i.e. $\mathrm{Tr}_F[\mathcal{E}(\rho_C \otimes \rho_D)] \neq \mathrm{Tr}_F[\mathcal{E}(\rho'_C \otimes \rho_D)]$. Often it is more convenient to formally define no-signalling relations of quantum channels. The negation of the just given operational statement, was in Ref. [16] shown to be equivalent, amongst other operational statements, to the following definition, which will be particularly convenient to work with in this thesis.

Definition 3.6 (No-signalling in channel): *Given a channel $\mathcal{E} : \mathcal{L}(\mathcal{H}_A \otimes \mathcal{H}_C) \to \mathcal{L}(\mathcal{H}_B \otimes \mathcal{H}_D)$, write $A \nrightarrow^s D$, say 'A* does not signal *to D', if and only if there exists a quantum channel $\mathcal{M} : \mathcal{L}(\mathcal{H}_C) \to \mathcal{L}(\mathcal{H}_D)$, with CJ representation $\rho^{\mathcal{M}}_{D|C}$ such that* $\mathrm{Tr}_B[\rho^{\mathcal{E}}_{BD|AC}] = \rho^{\mathcal{M}}_{D|C} \otimes \mathbb{1}_{A^*}$.

However, in a quantum channel, at least how it is commonly interpreted as describing the evolution of quantum systems at an earlier time to a later time, a lot of causal constraints are already fixed, namely that none of the later systems can then be causes of the earlier systems. As emphasised in many works, in particular by Leifer and Spekkens in Ref. [78], what appears as a prerequisite for developing a quantum generalisation of classical causal models is a formalism with which causally distinct situations, such as a joint state of two quantum systems at the same time and a channel from one system to another, can be represented mathematically on an equal footing — it should always be the same sort of object that is then constrained by different DAGs as causal structure. The next section will introduce the process formalism, which is one way to provide such a stage. Sec. 3.2.4 will then resume the current overview with the two remaining groups of works. Crucially, the process formalism does not necessarily lead to an interventionist account of causation and will also provide the stage for the treatment of quantum causal models in this thesis.

[11] While this is not the notion of causal relations that underlies Pearl's presentation of classical causal models in Ref. [9] (see Sec. 3.1.2), nor in Refs. [111, 112], many understand classical causal models in such a light. It is one thing to note the role of interventions in giving causal relations operational meaning, and another to *define* causal relations in terms of interventions.

3.2.3 Intermezzo: the process formalism

This section introduces a central concept for this thesis, that of a *quantum process operator*. Up to the different convention for the CJ isomorphism in this thesis, a quantum process operator essentially is a process matrix as first defined by Oreshkov, Costa and Brukner in Ref. [43]. The below presentation of the formalism of quantum processes[12] will follow that in Ref. [3]. Historically, in Ref. [43] process matrices were introduced in order to study the conceivable ways in which an 'indefinite causal order' of events could be compatible with quantum theory without running into logical paradoxes. An introduction into the motivation for such inquiry, how it leads to the process formalism and the seminal findings in a large set of works since, is postponed to Sec. 7.1. Here, the set-up is introduced merely to: (1) provide a way to represent quantum data such that it does not already manifestly depend on the causal structure and (2) makes it possible to consider arbitrary quantum interventions and make predictions for their outcomes — for the time being, disregarding questions on 'indefinite causality'. The process formalism is a prerequisite for the continuation of the overview on quantum causal models in Sec. 3.2.4, for formulating the notion of a causal model this thesis studies, as well as it will ensure a smooth transition into the contents of Chap. 7 that will finally be concerned with 'indefinite causality'.

Quantum processes have many cousins in preceding and closely related formalisms: from the *multi-time formalism* [113–117], via *quantum combs* [32, 118], more general *quantum higher-order maps* [42, 67], to the almost identical *process matrices* [43, 48, 49, 53]. While these different works stem from distinct intentions and study distinct questions, they share that a system or locus of intervention is represented by a pair of Hilbert spaces, one representing the causal past — seen locally — and one representing the causal future. Some of the mentioned works are manifestly operational and associate these 'pairs of Hilbert spaces' with the 'before and after' of an intervention, while others leave them more abstract or may associate the pair of spaces with a single system to represent pre- and post-selected information about that system. To a certain degree, different perspectives will also feature in the remainder, however, here we choose to introduce them as the most general kind and under neutral terminology, which is also natural for the context of causal models: A *quantum node A* is a pair of an input system $\mathcal{H}_{A^{\text{in}}}$ and an output system $\mathcal{H}_{A^{\text{out}}}$. An *intervention at the node A* that maps the states of the incoming system to the states of the outgoing system, is modeled by a quantum instrument of the

[12] Note that this is not to be confused with the same terminology in the context of seeing quantum theory as a process theory (see, e.g., Ref. [24]), where 'quantum processes' are CP maps.

form $\{\mathcal{E}^{k_A}\}_{k_A}$, where the CP maps $\mathcal{E}^{k_A} : \mathcal{L}(\mathcal{H}_{A^{\rm in}}) \to \mathcal{L}(\mathcal{H}_{A^{\rm out}})$ are represented by

$$\tau_A^{k_A} := \left(\rho^{\mathcal{E}^{k_A}}_{A^{\rm out}|A^{\rm in}}\right)^T \ , \tag{3.6}$$

which is an operator on $\mathcal{H}_{A^{\rm in}} \otimes \mathcal{H}^*_{A^{\rm out}}$ (recalling our definition of CJ operators and that a Hilbert space $\mathcal{H}$ is assumed to be finite-dimensional and hence $\mathcal{H}$ is canonically isomorphic to $(\mathcal{H}^*)^*$).

In case of a deterministic intervention at node A with just one possible outcome — or equivalently the effective CPTP map from summing over all possible outcomes of an arbitrary quantum instrument — is denoted τ_A. For a set of quantum nodes $A_1, \ldots, A_n$, the *process* 'external to the nodes' is then most generally described by a *quantum process operator*[13].

Definition 3.7 (Quantum pocess operator): *A quantum process operator $\sigma_{A_1 \ldots A_n}$ (process operator for short) over the quantum nodes $A_1, \ldots, A_n$ is a positive semi-definite operator*

$$\sigma_{A_1 \ldots A_n} \in \mathcal{L}\Big(\bigotimes_{i=1}^{n} \mathcal{H}_{A_i^{in}} \otimes \mathcal{H}^*_{A_i^{out}}\Big) \ ,$$

such that for all sets of channels $\{\tau_{A_i}\}$ at the n nodes it holds that

$$\mathrm{Tr}\Big[\sigma_{A_1 \ldots A_n}\Big(\tau_{A_1} \otimes \ldots \otimes \tau_{A_n}\Big)\Big] = 1 \ .$$

As mentioned above, a process operator is the same as a process matrix as defined in Ref. [43], modulo the different choice of CJ representation that ensures the process operator to be a basis-independent object.

Given a process operator $\sigma_{A_1 \ldots A_n}$ and a choice of intervention at each node, $\tau_{A_i}^{k_{A_i}}$ with $i = 1, ..., n$, the joint probability distribution over the n outcomes is given by

$$P(k_{A_1}, \ldots, k_{A_n}) = \mathrm{Tr}\Big[\sigma_{A_1 \ldots A_n}\Big(\tau_{A_1}^{k_{A_1}} \otimes \ldots \otimes \tau_{A_n}^{k_{A_n}}\Big)\Big] \ . \tag{3.7}$$

It follows from Def. 3.7 that the expression on the right-hand side of Eq. (3.7) indeed defines a correctly normalised probability distribution $P(k_{A_1}, \ldots, k_{A_n})$ over all possible outcomes of the n interventions. Note that the reason for representing CP maps of interventions with $\tau_A^{k_A}$, the transpose of the CJ operator, rather than the latter itself, is so that Eq. (3.7) would take this form of a simple trace rule.

Importantly, and as is not hard to see, Def. 3.7 implies that for a process operator

[13] This definition agrees with the presentation in Ref. [3], while the one in Ref. [1] differs slightly in that it does not allow arbitrary quantum nodes as done here and that the labelling of the 'out' Hilbert space and its dual is the reverse compared to here.

$\sigma_{A_1 \dots A_n}$ it holds that

$$\mathrm{Tr}_{A_1^{\mathrm{in}} \dots A_n^{\mathrm{in}}} \left[\sigma_{A_1 \dots A_n} \right] = \mathbb{1}_{(A_1^{\mathrm{out}})^*} \otimes \dots \otimes \mathbb{1}_{(A_n^{\mathrm{out}})^*} \ . \tag{3.8}$$

Hence, it follows that a process operator $\sigma_{A_1 \dots A_n}$, seen as a CJ operator, also defines a channel from the output spaces of all nodes to the input spaces of all nodes,

$$\mathcal{P} : \mathcal{L}(\mathcal{H}_{A_1^{\mathrm{out}}} \otimes \dots \otimes \mathcal{H}_{A_n^{\mathrm{out}}}) \ \to \ \mathcal{L}(\mathcal{H}_{A_1^{\mathrm{in}}} \otimes \dots \otimes \mathcal{H}_{A_n^{\mathrm{in}}}) \ . \tag{3.9}$$

Eq. (3.7) can then be read as the composition of this channel $\mathcal{P}$ 'in a loop' with the CP maps of the interventions. Note that however not all channels of the form as in Eq. (3.9) define process operators. Furthermore, Eq. (3.7) also makes evident that a process operator $\sigma_{A_1 \dots A_n}$ defines a multi-linear map that maps tuples of n CP maps into the probabilities and can be seen as a special case of a higher-order map [67]. Just as we will often write 'given a channel $\rho_{C|B}$' by stating the CJ operator $\rho_{C|B}$ of the channel, we will often write 'given a quantum process $\sigma_{A_1 \dots A_n}$' by stating the process operator $\sigma_{A_1 \dots A_n}$. Alternative conditions to characterise process operators can be found in Refs. [43, 48, 49] (also see Sec. 7.1).

An important convention will be that if labels of quantum nodes appear on CJ operators of channels then we have suppressed the 'in' and 'out' to avoid clutter and write, e.g., $\sigma_{A_1 \dots A_n} = \rho^{\mathcal{P}}_{A_1 \dots A_n | A_1 \dots A_n}$, that is, the label A of a node refers to the respective output space A^{out} if A appears to the right of the 'bar' and to the input space A^{in} if it appears to the left of the 'bar'.

The way in which, for instance, a state ρ_{AB} of two systems A and B at the same time and a channel $\rho_{B|A}$ from A to B, which evolves state ρ_A forward, can be represented in a unified way in terms of process operators is by formally considering A and B as two quantum nodes, for which $\mathcal{H}_{A^{\mathrm{out}}} = \mathcal{H}_{A^{\mathrm{in}}} = \mathcal{H}_A$ and $\mathcal{H}_{B^{\mathrm{out}}} = \mathcal{H}_{B^{\mathrm{in}}} = \mathcal{H}_B$. In the first case the process operator is given by $\sigma_{AB} = \mathbb{1}_{(A^{\mathrm{out}} B^{\mathrm{out}})^*} \otimes \rho_{AB}$, and in the second case by $\sigma'_{AB} = \mathbb{1}_{(B^{\mathrm{out}})^*} \otimes \rho_{B|A} \otimes \rho_A$. Following the convention from Sec. 2.2 for suppressing identity operators, these are more conveniently written as $\sigma_{AB} = \rho_{AB}$ and $\sigma'_{AB} = \rho_{A|B} \ \rho_B$, respectively . Alternatively, any channel $\rho_{CD|AB}$ from quantum systems AB to CD itself already is a special case of a process operator, simply by seeing A and B as quantum nodes with trivial input spaces and C and D as quantum nodes with trivial output spaces.

Some more notational conventions will be useful. If $S = \{A_1, \dots A_n\}$ is a set of quantum nodes, then we let 'local interventions at S', denoted by $\tau_S^{k_S}$, refer to an intervention at each node individually, $\tau_S^{k_S} = \tau_{A_1}^{k_{A_1}} \otimes \dots \otimes \tau_{A_n}^{k_{A_n}}$ with k_S standing for the tuple of outcomes. More generally, interventions $\tau_S^{k_S}$ at S that are not of that form are referred to as global interventions. For a set of nodes S let $\mathcal{H}_{S^{\text{in}}} := \bigotimes_{A\in S}\mathcal{H}_{A^{\text{in}}}$ and $\mathcal{H}_{S^{\text{out}}} := \bigotimes_{A\in S}\mathcal{H}_{A^{\text{out}}}$. It will be convenient to use the short-hand notation $\text{Tr}_A[\ldots] := \text{Tr}_{A^{\text{in}}(A^{\text{out}})^*}[\ldots]$, as a 'partial trace over node A'. Similarly, $\text{Tr}_S[\ldots] := \text{Tr}_{S^{\text{in}}(S^{\text{out}})^*}[\ldots]$ for S a set of nodes. This is particularly handy when considering *marginal processes*. Let $\sigma_{A_1\ldots A_n}$ be a quantum process, then for some choice of interventions τ_S at $S \subset \{A_1, \ldots A_n\}$ the marginal process on the remaining nodes $R := \{A_1, \ldots A_n\} \setminus S$ will in general depend on the choice τ_S and is denoted $\sigma_R^{\tau_S} := \text{Tr}_S[\sigma_{A_1\ldots A_n}\ \tau_S]$.

Since the quantum nodes $A_1, \ldots, A_n$ can in particular be regarded as loci of interventions, where one may imagine an agent to be stationed and able to perform arbitrary quantum instruments, given a quantum process $\sigma_{A_1\ldots A_n}$, one can then naturally consider the condition of no-signalling between subsets of nodes.

Definition 3.8 (No-signalling between nodes of a quantum process [49]): *Given a quantum process $\sigma_{A_1\ldots A_n}$, for disjoint subsets $S, T \subseteq \{A_1, \ldots, A_n\}$ say* the nodes S cannot signal to the nodes T, *write $(S \not\to^s T)_{\sigma_{STR}}$, where $R := \{A_1, \ldots, A_n\} \setminus (S \cup T)$, if and only if for all interventions $\tau_T^{k_T}$ at T and all interventions τ_R at R the probability distribution $p(k_T|\tau_S) = \text{Tr}\big[\sigma_{STR}\big(\tau_S \otimes \tau_T^{k_T} \otimes \tau_R\big)\big]$ is independent from the choice of intervention τ_S at S.*

The signalling properties of processes will be further studied in Sec. 5.7. Due to the present focus on processes compatible with a 'definite causal order' it may be useful to point out more precisely the link to the closely related formalism of *quantum combs*, as defined in Ref. [32], where it was used to formalise the study of quantum networks. A $(n+1)$-comb can be seen to be a multi-linear map that maps CP maps at n quantum nodes $A_1, \ldots, A_n$ into a CP map of the form $\mathcal{L}(\mathcal{H}_I) \to \mathcal{L}(\mathcal{H}_O)$, subject to conditions that relate the total order of nodes, as enumerated by $A_1, \ldots, A_n$, to certain no-signalling relations. In case the output CP map of the comb has trivial input and output systems I and O, the comb maps into the probabilities and becomes a special case of a quantum process: a quantum process $\sigma_{A_1\ldots A_n}$ over n quantum nodes is a quantum comb for the given total order of its nodes (as enumerated by $A_1, \ldots, A_n$) if and only if

$$\sigma_{A_1\ldots A_n} \;=\; \frac{1}{d_{A_n^{\text{out}}}} \text{Tr}_{(A_n^{\text{out}})^*}[\sigma_{A_1\ldots A_n}] \otimes \mathbb{1}_{(A_n^{\text{out}})^*} \tag{3.10}$$

and $\forall l = 1, \ldots, n-1$

$$\text{Tr}_{A_{l+1}\ldots A_n}[\sigma_{A_1\ldots A_n}] = \frac{1}{d_{A_l^{\text{out}}}} \text{Tr}_{(A_l^{\text{out}})^*}\Big[\text{Tr}_{A_{l+1}\ldots A_n}[\sigma_{A_1\ldots A_n}]\Big] \otimes \mathbb{1}_{(A_l^{\text{out}})^*}\ . \tag{3.11}$$

It is immediate that if a quantum process $\sigma_{A_1 \dots A_n}$ is a comb for the total order of nodes $A_1, \dots, A_n$, then for any $i \leq j < k \leq l$ the set of nodes $A_k, A_{k+1}, \dots A_l$ cannot signal to the set of nodes $A_i, A_{i+1}, \dots A_j$. Signalling is thus possible at most to nodes later in the total order.

Further intuition for quantum processes will be developed in the remainder of the thesis.

3.2.4 Previous approaches II

This section will continue where Sec. 3.2.2 left the overview on previous approaches to quantum causal models. As remarked there, it is a strong desideratum for a definition of quantum causal models to have the feature of 'predictiveness for arbitrary interventions'. Now, a quantum process $\sigma_{A_1 \dots A_n}$ over quantum nodes $A_1, \dots, A_n$, as introduced in Sec. 3.2.3, is a fully quantum object that allows to consider and make predictions for arbitrary interventions at $A_1, \dots, A_n$. If it furthermore is a quantum comb as defined in Ref. [32], that is, it satisfies the conditions from Eqs. (3.10) and (3.11), in particular then $A_1, \dots, A_n$ can be seen to have a fixed causal order[14]. A fourth sense in which the term 'quantum causal model' has been used in the literature then essentially coincides with the notion of a quantum comb, reducing a causal model to the predictiveness aspect. This group includes for instance Ref. [119, 120].

Importantly, a core aspect of a causal model framework, as understood in this thesis, but that the just mentioned usage of the term ignores, is that it is supposed to be a formalisation of how to give *causal explanations*. This aims at the capability to answer questions, such as, what the causal structure of the quantum nodes of a quantum process $\sigma_{A_1 \dots A_n}$ is and when and based on what assumptions can one assert that no common causes are omitted in the choice of quantum nodes under study?

A fifth and last approach in the overview then is the first instance of a framework of quantum causal models that is in the interventionist tradition, equating causation with signalling, but also in keeping with the spirit of classical causal models in that it formulates a quantum Markov condition and is explicitly concerned with giving causal explanations. This is the notion of a quantum causal model as proposed by Costa and Shrapnel in Ref. [82] (also see Ref. [121]). It focuses on two concepts, 'interventions' and 'autonomous causal mechanisms'. Concerning the former, predictiveness for arbitrary interventions is again built in by virtue of that a quantum causal model in particular specifies a quantum process. Concerning the latter, a 'causal mechanism' that the arrow in a DAG of a causal model is supposed to stand

[14] This does not exhaust the cases when one can regard that to be the case, however, a discussion of the corresponding concept of 'causal separability' is postponed to Sec. 7.1.1.

for, is taken to mean the passing of a quantum system, which mediates the signalling as a physical process — a feature that is shared with the approaches in group two from Sec. 3.2.2.

On that basis, Ref. [82] defined a quantum causal model by specifying a DAG G with vertices $A_1, \ldots, A_n$ and a quantum process $\sigma_{A_1 \ldots A_n}$ over quantum nodes $A_1, \ldots, A_n$ with the special property that each output space A_i^{out} factorises into as many subsystems as the vertex A_i has children in the DAG G, i.e. A_i^{out} is required to have subsystems $A_i^{(j)}$ with $A_j \in Ch(A_i)$, and such that $\sigma_{A_1 \ldots A_n}$ satisfies their proposed notion of a quantum Markov condition relative to G. The latter condition then demands that $\sigma_{A_1 \ldots A_n} = \bigotimes_{j=1}^{n} \rho_{A_j|Pa(A_j)}$, where each $\rho_{A_j|Pa(A_j)}$ represents a channel $\mathcal{L}(\bigotimes_{A_i \in Pa(A_j)} \mathcal{H}_{A_i^{(j)}}) \to \mathcal{L}(\mathcal{H}_{A_j^{in}})$. In particular the Bell scenario described in Sec. 3.2.1 fits into that picture, seeing as the corresponding process is of the form $\sigma_{ABC} = \rho_{B|A^{(B)}} \otimes \rho_{C|A^{(C)}} \otimes \rho_{A^{(B)}A^{(C)}}$, where $\rho_A = \rho_{A^{(B)}A^{(C)}}$ is a Bell state and the channels $\rho_{B|A^{(B)}}$ and $\rho_{C|A^{(C)}}$ describe the sending of the subsystems $A^{(B)}$ and $A^{(C)}$ into the respective space-like separated regions.

The approach from Ref. [82] also facilitated quantum analogues of other aspects of classical causal models such as a notion of faithfulness and moreover led to the development of a quantum causal discovery algorithm [82, 121] (also see Sec. 5.7.3). In the view that takes causation to be signalling and common causes necessarily to be composite systems with a subsystem 'per causal relation', the framework from Ref. [82] appears as an interesting and plausible approach. There are however reasons why one might not be fully satisfied with such an approach.

First, independently from the definition of a causal model, and also independently from one's preference concerning whether or not it is desirable to have causal relations as an agent based, interventionist notion or not, *defining* a causal relation as signalling comes with an oddity. The possibility to signal can only be a property that obtains given certain data. For the case of quantum processes this discussion is postponed to Sec. 5.7.1, but the claimed oddity essentially boils down to the following observation just for 'ordinary' quantum channels. Given a channel $\rho_{B_1 \ldots B_k|A_1 \ldots . A_n}$, suppose that A_i cannot signal to B_j and also not to B_m for $j \neq m$. Note that it however may still be the case that A_i can signal to the composite system $B_j B_m$[15]. While the possibility to signal should arguably lead to the conclusion of

[15] A simple example of such a situation can be given even in purely classical terms. Let X, Y and Z be bits and $P(Y, Z|X)$ the classical channel that arises from a functional model as follows: there is an additional bit λ and it holds that $Y = X + \lambda \bmod 2$ and that $Z = \lambda$, as well as, suppose $P(Y, Z|X)$ arises from marginalising over λ for the uniform distribution $P(\lambda = 0) = 1/2 = P(\lambda = 1)$. It is straightforward to verify that while X can signal to $Y \times Z$, it cannot signal to Z alone and also not to Y alone, since the output of the marginal channel $P(Y|X)$ is the uniform distribution over Y independently from X.

a causal relation on any account, a definition is an 'if and only if' relation and if defining causation as signalling, one would have to conclude that A_i is *not* a 'direct cause' of B_j given that A_i cannot signal to B_j. This however is an assertion one does not quite know what to make of, given that A_i would also not be a 'direct cause' of B_m, while it is a 'direct cause' of B_jB_m. It is an assertion that is at odds with taking DAGs as representing individually meaningful direct cause relations, where in particular their absences matter (also see Sec. 4.1). Now, it is true that in case of a quantum causal model as defined in Ref. [82] this issue does not arise, that is, the DAG can be trusted also concerning the absences of arrows it encodes (see Sec. 5.7), however, then the notion of a causal relation cannot be distentangled from the notion of a causal model. This in turn is particularly pertinent given the following point.

Second, no justification has been given why the definition of a quantum causal model in Ref. [82] should be the most general one. Indeed, the assumption of 'composite systems as common causes' does not seem to exhaust the cases, where one would like to be able to give a causal account of a quantum channel, or generally a quantum process, in terms of common causes. This insight was gained in the work by Allen *et al.* in Ref. [4] by moving away from an interventionist account of causation. This work will be sketched in the subsequent section and provides the basis for this thesis.

3.2.5 The work by Allen *et al.* and causal principles

The works discussed in the previous sections left unanswered the question of what an appropriate notion of quantum causal models is that incorporates all the mentioned desirable features, but can deal with the most general case and has a conceptually clear grounding. In order to arrive at such, one is well-advised to first properly understand the arguably most basic situation of causal reasoning — the common cause scenario, with which it all began in Sec. 3.2.1. This is what Allen *et al.* undertook and studied in detail in Ref. [4], taking inspiration from the analysis of classical causal models in Sec. 3.1.2. If classical causal models got something right about causal reasoning for classical variables, then this manifests itself in, or in fact can be seen as a generalisation of, Reichenbach's common cause principle. Hence, what is needed is a common cause principle in intrinsically quantum terms. The hope that this might be possible was already expressed in Ref. [13]. The 'blueprint' for causal models, which the analysis of the classical case in Sec. 3.1.2 may be seen to constitute is this: provided a precise definition of causal relations, one may then be able to obtain the principle as a theorem rather than an ad-hoc assertion, and in a second step generalise from the common cause scenario to arbitrary DAGs.

The following summarises the ideas and results from Ref. [4]. This is presented in a slightly different way than in Ref. [4], in accordance with that 'blueprint' from Sec. 3.1.2: here causal principles are formulated explicitly to match the analogy, which did not appear literally in Ref. [4], but are conceptually entirely contained in Ref. [4]. The approach in Ref. [4] involves in particular the proposal of a different take on causal relations compared to the approaches in Secs. 3.2.2 and 3.2.4, which will be introduced here to the extent it was covered in Ref. [4]. A corresponding fully general definition of causal structure was first given in our work in Ref. [1] and will be presented in Chap. 4.

3.2.5.1 The quantum common cause principle

Let B and C be quantum systems. They could in general be causally unrelated or stand in one of the five possible causal relationships already described for the classical case in Sec. 3.1.2, i.e. B could be a cause of C, vice versa, there could be a common cause A or a combination of the latter with one of the former two. Now, suppose A is a complete common cause of B and C, as depicted in Fig. 3.5, i.e. in particular B and C are not causes of each other.

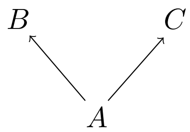


Figure 3.5: A is the complete common cause of B and C.

An analogous treatment to that in Sec. 3.1.2 has to answer the two questions what the object is that is constrained by such an assertion and what the constraint is. The proposal from Ref. [4] for the first is that the quantum analogue of the classical channel $P(Y, Z|X)$ is a quantum channel $\mathcal{E} : \mathcal{L}(\mathcal{H}_A) \rightarrow \mathcal{L}(\mathcal{H}_B \otimes \mathcal{H}_C)$ that describes the evolution from A to B and C. Concerning the second, the constraint imposed by the asserted causal scenario is that the CJ operator of the channel factorises as

$$\rho_{BC|A} \;=\; \rho_{B|A}\; \rho_{C|A}\;. \tag{3.12}$$

The constraint $\rho_{BC|A} = \rho_{B|A}\; \rho_{C|A}$ looks analogous to the one in Reichenbach's common cause principle, that is, $P(Y, Z|X) = P(Y|X)P(Z|X)$. It is of course a generalisation, containing the classical one as a special case for a preferred product basis of $\mathcal{H}_A$, $\mathcal{H}_B$ and $\mathcal{H}_C$, relative to which $\rho_{BC|A}$ is diagonal and encodes the conditional distribution $P(Y, Z|X)$ on its diagonal (see Sec. 5.3 for a detailed analysis). For two such diagonal operators $\rho_{B|A}$ and $\rho_{C|A}$ commutation is trivial. Commutation is also trivial if $\mathcal{H}_A$ has subsystems corresponding to tensor factors, $\mathcal{H}_A = \mathcal{H}_{A^{(B)}} \otimes \mathcal{H}_{A^{(C)}}$ such that $\rho_{B|A} = \rho_{B|A^{(B)}} \otimes \mathbb{1}_{A^{(C)*}}$ and $\rho_{C|A} = \mathbb{1}_{A^{(B)*}} \otimes \rho_{C|A^{(C)}}$, i.e. $\rho_{BC|A} = \rho_{B|A^{(B)}} \otimes \rho_{C|A^{(C)}}$. This could be seen as the 'complete common cause scenario' according to Ref. [82] (see Sec. 3.2.4).

However, the proposed principle is more general. It demands a factorisation as in Eq. (3.12), but where $\rho_{B|A}$ and $\rho_{C|A}$ are allowed to act non-trivially on A without a global factorisation of A. Note that the hermiticity of $\rho_{BC|A}$ still implies that the factors commute, $[\rho_{B|A}, \rho_{C|A}] = 0$ [4].

An instructive example, presented in Ref. [4], is the incoherent copy channel $\rho_{BC|A}$ that describes a situation, where qubit A is measured in the computational basis $|0\rangle, |1\rangle$ and, depending on the outcome $i = 0, 1$, the qubits B and C are prepared in state $|i\rangle|i\rangle$. The CJ operator is given by $\rho_{BC|A} = |000\rangle\langle 000|_{BCA^*} + |111\rangle\langle 111|_{BCA^*}$ and can be verified to indeed be of the form $\rho_{BC|A} = \rho_{B|A}\ \rho_{C|A}$ [4]. Here A does not factorise into subsystems, which independently go to B and C; system A is a qubit with a prime-dimensional Hilbert space. Nonetheless, one would want to be able to say that A is the complete common cause of B and C, seeing as it is a quantum version of the classical copy map — the maybe canonical example for a common cause explanation.

Since useful later, the formal statement of the principle is given for a slightly more general case.

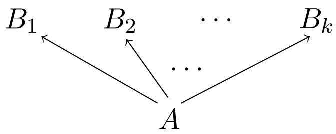


Figure 3.6: A is the complete common cause of $B_1, \ldots, B_k$.

Principle 2 (Quantum common cause principle): *If system A is the* complete common cause *of systems $B_1, \ldots, B_k$ as shown in Fig. 3.6 then the channel $\rho_{B_1 \ldots B_k|A}$ that describes their evolution, factorises as*

$$\rho_{B_1 \ldots B_k|A} = \prod_{i=1}^{k} \rho_{B_i|A} \ , \tag{3.13}$$

such that the marginal channels commute pairwise, $[\rho_{B_i|A}, \rho_{B_j|A}] = 0\ \forall i, j$.

Note that in this case the pairwise commutation of the k factors is not implied by the factorisation itself, but rather is an additional, substantial condition. In a similar spirit as in Sec. 3.1.2, this begs the question why one should hold this principle to be a reasonable one, be it for just two systems B and C, or for k systems. The answer offered in Ref. [4] starts from proposing causal relations as relations of influence between quantum systems in underlying unitary transformations. This is most conveniently formalised by defining the *no-influence* condition:

Definition 3.9 (No-influence in unitary transformation): *Given a unitary transformation $U : \mathcal{H}_A \otimes \mathcal{H}_C \rightarrow \mathcal{H}_B \otimes \mathcal{H}_D$ with CJ representation $\rho^U_{BD|AC}$, write $A \nrightarrow D$, say 'A* does not influence *D', if and only if there exists a quantum channel $\mathcal{M}$: $\mathcal{L}(\mathcal{H}_C) \rightarrow \mathcal{L}(\mathcal{H}_D)$, with CJ representation $\rho^{\mathcal{M}}_{D|C}$ such that $\mathrm{Tr}_B[\rho^{\mathcal{U}}_{BD|AC}] = \rho^{\mathcal{M}}_{D|C} \otimes \mathbb{1}_{A^*}$.*

The effective description with a channel $\rho_{B_1 \ldots B_k|A}$ is thought to arise from the evolution with an underlying unitary transformation U that involves these systems, but in general also further input and output systems. Now, if A is the complete common cause of $B_1, \ldots, B_k$ as in Fig. 3.6, then A must be the only input system that influences more than one of the output systems $B_1, \ldots, B_k$. Hence, U may involve at most further 'local disturbances' $\lambda_1, \ldots, \lambda_k$ as input systems, in much the same fashion as for the classical case in Sec. 3.1.2. More formally,

Definition 3.10 (Compatibility with complete common cause [4]): *Given a channel $\rho_{B_1 \ldots B_k|A}$, it is* compatible *with A being the complete common cause of $B_1, \ldots, B_k$ if and only if there exist k auxiliary systems λ_i and a unitary channel $\rho^U_{B_1 \ldots. B_k F|A \lambda_1 \ldots \lambda_k}$ such that*

(1) *for some product state $\rho_{\lambda_1} \otimes \cdots \otimes \rho_{\lambda_n}$ it holds that*

$$\rho_{B_1 \ldots B_k|A} = \mathrm{Tr}_F \overline{\mathrm{Tr}}_{\lambda_1 \ldots \lambda_n} \left[\rho^U_{B_1 \ldots. B_k F|A \lambda_1 \ldots \lambda_k} \left(\rho_{\lambda_1} \otimes \cdots \otimes \rho_{\lambda_n} \right) \right] , \quad (3.14)$$

(2) *the unitary U satisfies the no-influence conditions $\{\lambda_i \nrightarrow B_j\}_{j \neq i}$.*

The assumption that the 'local disturbances' $\lambda_1, \ldots, \lambda_k$ can be ascribed a product state when A is the complete common cause parallels the corresponding assumption in the classical case concerning statistically independent local disturbances. See Sec. 5.2.4 for a discussion of why no attempt is made to further justify this assumption. The main result from Ref. [4] then is:

Theorem 3.4 (Equivalent statements for complete common cause scenario [4]): *Given a channel $\rho_{B_1 \ldots B_k|A}$, the following statements are equivalent:*

(1) *The channel $\rho_{B_1 \ldots B_k|A}$ is compatible with A being the complete common cause of $B_1, \ldots, B_k$.*

(2) *The channel* $\rho_{B_1 \ldots B_k|A}$ *factorises as* $\rho_{B_1 \ldots B_k|A} = \prod_{i=1}^{k} \rho_{B_i|A}$*, where the corresponding marginal channels commute pairwise, i.e.* $\forall i, j$, $[\rho_{B_i|A}, \rho_{B_j|A}] = 0$.

On the basis of taking causal relations as relations of influence in underlying unitary evolution, whenever A is the complete common cause of $B_1, \ldots, B_k$, Principle 2 necessarily has to be satisfied, provided the product state assumption. In that sense Thm. 3.4 may therefore be taken as a justification of the principle.

Note that, unlike the incoherent copy channel mentioned above, the coherent version defined by mapping $|0\rangle_A \mapsto |00\rangle_{BC}$ and $|1\rangle_A \mapsto |11\rangle_{BC}$ defines a channel, the CJ operator of which does not factorise as in Eq. (3.12), i.e. $\rho_{BC|A} \neq \rho_{B|A}\ \rho_{C|A}$ [4]. This is just as one would expect on the basis of causal relations as influence in underling unitary evolution because a unitary transformation that implements the coherent copy map will involve further common causes to B and C and hence the factorisation condition should indeed fail to detect that very fact [4].

3.2.5.2 General quantum causal principle

Based on the result of Thm. 3.4, Allen *et al.* in Ref. [4] proposed a definition of quantum causal models in accordance with the quantum common cause principle. The presentation of the proposal here will adopt the scheme from Sec. 3.1.2: first formulate the general quantum causal principle that generalises the quantum common cause principle to arbitrary causal scenarios as represented by a DAG, in analogy to how the classical Principle 1 generalises Reichenbach's common cause principle.

For the complete common cause case the constraint concerned a channel $\rho_{B_1 \ldots B_k|A}$, which is natural since none of the $B_1, \ldots, B_k$ are, by assumption, causes of each other. Now allowing arbitrary causal relations between a set of quantum systems — as long as expressible by a DAG — the kind of object with which the quantum systems can always be described, and that is constrained by causal structure, is a quantum process operator. However, in Refs. [1, 4] it is not any kind of quantum nodes that are allowed as the vertices of a causal DAG, but a special kind[16]:

Definition 3.11 (Quantum $i$node): *A* quantum $i$node A *is a quantum node with isomorphic input and output systems,* $\mathcal{H}_{A^{in}} \cong \mathcal{H}_{A^{out}}$*, where for convenience we let them be copies of each other,* $\mathcal{H}_{A^{out}} = \mathcal{H}_{A^{in}}$.

The decisive feature of a quantum $i$node A is that it then is always possible to consider 'no intervention' at A. This is represented by the identity channel, the

[16] The terminology of an $i$node is not established in the literature, but introduced here for ease of reference given that in this thesis both will be needed, the general formalism of processes with arbitrary quantum nodes, as well as, the restricted ones.

special intervention τ_A^{id}, which is nothing but the 'linking operator' from the CJ isomorphism in Sec. 2.2. If the input and output spaces of a quantum node have different dimension, then a 'non-trivial' intervention necessarily has to happen at the respective locus, in order to mediate the input system to the output system. A restriction to quantum $i$nodes aims at a framework concerned with the causal relations between quantum systems, rather than 'labs' or interventionist interpretations otherwise of quantum nodes. See Sec. 4.2 for further discussion.

In analogy to the classical Principle 1, the following then suggests itself by virtue of Principle 2 from the complete common cause scenario.

Principle 3 (Quantum causal principle): *Given quantum inodes $A_1, \ldots, A_n$, if their causal structure is as in the DAG G with vertices $A_1, \ldots, A_n$, with no common causes missing, then the process operator $\sigma_{A_1 \ldots A_n}$ describing these quantum inodes admits a factorization into pairwise commuting CJ operators of channels of the form $\sigma_{A_1 \ldots A_n} = \prod_{i=1}^n \rho_{A_i|Pa(A_i)}$.*

This in turn suggests — in keeping with the causal principle — the following definition of a quantum causal model, proposed in Ref. [4].

Definition 3.12 (Quantum causal model): *A* Quantum causal model *(QCM) is given by:*

(1) *a causal structure represented by a DAG G with vertices corresponding to quantum inodes $A_1, ..., A_n$,*

(2) *for each A_i, a quantum channel $\rho_{A_i|Pa(A_i)} \in \mathcal{L}(\mathcal{H}_{A_i^{in}} \otimes \mathcal{H}^*_{Pa(A_i)^{out}})$ such that for all i, j, $[\rho_{A_i|Pa(A_i)}\ ,\ \rho_{A_j|Pa(A_j)}] = 0$.*

The quantum causal model defines a process operator over the quantum inodes $A_1, ..., A_n$ given by

$$\sigma_{A_1 \ldots A_n} = \prod_i \rho_{A_i|Pa(A_i)} \ . \tag{3.15}$$

As before with the common cause principle, this begs the question why would Principle 3 be justified? Why should Def. 3.12 be the right definition of a quantum causal model? Ref. [4] proposed the definition without further justification. A mere appealing to analogy with Principle 2 and that both involve a factorisation into pairwise commuting operators does not suffice for a framework that aspires to be the general one for causal reasoning about quantum systems. Of course, the intuition was that the story which justified Principle 2 should extend and allow a theorem to a similar effect as Thm. 3.4. It turns out this is not entirely trivial and will be the first main result in Chap. 5. The exploration of this framework of quantum causal models is then undertaken in the remainder of Chap. 5. Before that, Chapter 4 will first lay the foundation by formalising the suggested picture of quantum causal relations in full generality — the first achievement of this thesis proper.

Chapter 4

Quantum causal structure

This chapter presents the main concepts of this thesis, common to all three of our publications in Refs. [1–3] — the *quantum direct-cause relation* between quantum systems as one that inheres in unitary transformations, the notion of *causal structure* any unitary transformation thereby has, and how that notion lifts to the level of unitary processes over quantum nodes. It also states a fundamental link between causal relations of quantum systems and structural properties of the underlying Hilbert spaces — a tool that will feature heavily in most proofs throughout. This short chapter thus *serves to expose* the definitions and observations that form *the basis* of this thesis and the thread that runs through the subsequent chapters.

4.1 Causal structure of unitary transformations

The previous Section. 3.2.5 summarised the main achievement from Ref. [4], namely, the formulation of a quantum common cause principle and, roughly speaking, how it was turned from an ad-hoc assertion to a theorem. This relied on the no-influence condition from Def. 3.9: given a unitary transformation $U : \mathcal{H}_A \otimes \mathcal{H}_C \to \mathcal{H}_B \otimes \mathcal{H}_E$, say A *does not influence* E, written $A \nrightarrow E$, if and only if $\mathrm{Tr}_B[\rho^U_{BE|AC}] = \rho^{\mathcal{M}}_{E|C} \otimes \mathbb{1}_{A^*}$ for some marginal channel $\mathcal{M} : \mathcal{L}(\mathcal{H}_C) \to \mathcal{L}(\mathcal{H}_E)$. This condition is equivalent to $\mathrm{Tr}_B \circ \mathcal{U} = \mathrm{Tr}_A \otimes \mathcal{M}$ and expressed graphically in Fig. 4.1.

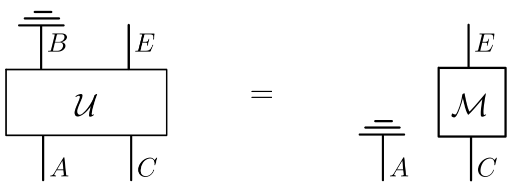


Figure 4.1: Graphical representation of $A \nrightarrow E$ for unitary channel $\mathcal{U}$.

The idea is, given a unitary map U, whenever there *is* influence from an input system to an output system, then this is *causal influence.*

Definition 4.1 (Direct cause relation): *Given a unitary transformation* $U : \mathcal{H}_A \otimes \mathcal{H}_C \to \mathcal{H}_B \otimes \mathcal{H}_E$*, system* C *is said to be a* direct cause *of* E*, written* $C \to E$*, if and only if* C *can influence* E*, i.e.* $\neg(C \nrightarrow E)$*.*

For a unitary transformation with a fixed tensor product structure of subsystems in both domain and codomain (not necessarily the same), one can then ask for each output system what its direct causes are.

Definition 4.2 (Causal parents in unitary transformation): *Given a unitary transformation* $U : \mathcal{H}_{A_1} \otimes \ldots \otimes \mathcal{H}_{A_n} \to \mathcal{H}_{B_1} \otimes \ldots \otimes \mathcal{H}_{B_k}$*, for* $j \in \{1, ..., k\}$ *the set*

$$Pa(B_j) \ := \ \{ \ A_i \mid i \in \{1, ..., n\}, \ A_i \to B_j \ \} \tag{4.1}$$

is called the causal parents *of output subsystem* B_j*.*

A crucial property of unitary channels is the consequence from causal relations observed by the following theorem.

Theorem 4.1 *Given a unitary transformation* $U : \mathcal{H}_{A_1} \otimes \ldots \otimes \mathcal{H}_{A_n} \to \mathcal{H}_{B_1} \otimes \ldots \otimes \mathcal{H}_{B_k}$ *with the family of causal parents* $\{Pa(B_j)\}_{j=1}^k$*, the CJ operator of the associated channel* $\rho^U_{B_1 \ldots B_k | A_1 \ldots . A_n}$ *factorises in the following way*

$$\rho^U_{B_1 \ldots B_k | A_1 \ldots . A_n} = \prod_{j=1}^{k} \rho_{B_j | Pa(B_j)} \ , \tag{4.2}$$

where for all $j, m = 1, ..., k$*, it holds that* $[\rho_{B_j | Pa(B_j)} \ , \ \rho_{B_m | Pa(B_m)}] = 0$*.*

Proof: Let $\rho^U_{B_1 \ldots B_k | A_1 \ldots . A_n}$ be the CJ representation of a unitary channel with family of causal parents $\{Pa(B_j)\}_{j=1}^k$. For $j \in \{1, \ldots, k\}$ let $\overline{B_j} := \{B_1, \ldots, B_k\} \backslash \{B_j\}$ and $\overline{Pa(B_j)} := \{A_1, \ldots, A_n\} \setminus Pa(B_j)$. By assumption, it holds that

$$\mathrm{Tr}_{\overline{B_j}} \left[\rho^U_{B_1 \ldots B_k | A_1 \ldots . A_n} \right] \ = \ \rho_{B_j | Pa(B_j)} \otimes \mathbb{1}_{(\overline{Pa(B_j)})^*} \ . \tag{4.3}$$

Let $\mathcal{H}_A := \bigotimes_{i=1}^n \mathcal{H}_{A_i}$, and observe that the channel $\rho^U_{B_1 \ldots B_k | A}$ is trivially compatible with A being the complete common cause of $B_1 \ldots B_k$ (see Def. 3.10), since it is its own dilation with trivial auxiliary systems λ_i. Theorem 3.4 then implies

$$\rho^U_{B_1 \ldots B_k | A_1 \ldots . A_n} \ = \ \rho^U_{B_1 \ldots B_k | A} \ = \ \prod_{j=1}^{k} \rho_{B_j | A} \ , \tag{4.4}$$

where the marginal channels on the right-hand side have to commute pairwise. Comparison with Eq. 4.3 yields that for every $j = 1, \ldots, k$,

$$\rho_{B_j|A} \;=\; \mathrm{Tr}_{\overline{B_j}}\left[\rho^U_{B_1 \ldots B_k|A}\right] \;=\; \rho_{B_j|Pa(B_j)} \otimes \mathbb{1}_{(\overline{Pa(B_j)})^*} \;, \tag{4.5}$$

hence, $\rho^U_{B_1\ldots B_k|A_1 \ldots .A_n} = \prod_{j=1}^k \rho_{B_j|Pa(B_j)}$, by our convention of suppressing identity operators. $\square$

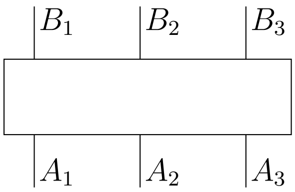
A first insight now ensues from asking, given $\rho^U_{B_1\ldots B_k|A_1 \ldots .A_n}$, what are the causal parents of, say the composite subsystem of B_j and B_m taken together (for $j \neq m$)? It is immediate from Thm. 4.1 that the marginal channel into $B_j B_m$ is of the form $\rho_{B_j|Pa(B_j)}\ \rho_{B_m|Pa(B_m)}$. Hence,

$$\forall j, m,\ j \neq m, \quad \big(\, A_i \nrightarrow B_j \quad \wedge \quad A_i \nrightarrow B_m \,\big) \quad \Rightarrow \quad A_i \nrightarrow B_j B_m \;. \tag{4.6}$$

The causal structure of a unitary transformation U naturally is the set of all causal relations between all subsets of subsystems — an exhaustive description of all the pathways of influence mediated by U. Due to the property in Eq. (4.6), this is completely specified by the causal parents of the single output systems.

Definition 4.3 (Causal structure of unitary transformation): *Given a unitary transformation $U : \mathcal{H}_{A_1} \otimes \ldots \otimes \mathcal{H}_{A_n} \rightarrow \mathcal{H}_{B_1} \otimes \ldots \otimes \mathcal{H}_{B_k}$ the family of causal parents $\{Pa(B_j)\}_{j=1}^k$ is called its* causal structure *and can be represented by a DAG with vertices $A_1, \ldots, A_n$ and $B_1, \ldots, B_k$ and an arrow from A_i to B_j whenever $A_i \in Pa(B_j)$.*

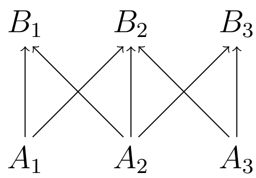
Fig. 4.2 shows an example of a unitary map and its causal structure. Note that in this case A_2 *is* the complete common cause of B_1 and B_3, that is, it is the kind of unitary which is asserted to exist by compatibility of a channel $\rho_{B_1 B_3|A_2}$ with A_2 being the complete common cause of B_1 and B_3.



(a)

$$\begin{aligned} Pa(B_1) &= \{A_1, A_2\}, \\ Pa(B_2) &= \{A_1, A_2, A_3\}, \\ Pa(B_3) &= \{A_2, A_3\}. \end{aligned}$$

(b)



(c)

Figure 4.2: Example of a causal structure: if the unitary U in (a) has the causal structure in (b), the latter can be represented as a DAG as in (c).

Why tie causal relations to unitary transformations?

An immediate question might be what is the difference between the condition that A cannot signal to E given an arbitrary channel $\rho_{BE|AC}$ (cf. Def. 3.6) and the relation of no-influence from A to E specifically for a unitary channel $\rho^U_{BE|AC}$ (cf. Def. 3.9). Mathematically speaking, the latter of course is just an instance of the former. In particular, this means that the no-influence relation inherits all the equivalent operational statements. Given a unitary channel $\rho^U_{BE|AC}$, that $A \nrightarrow E$ holds is, for instance, equivalent to that for all states ρ_C, the choice of state ρ_A makes no difference to the marginal state $\text{Tr}_B\overline{\text{Tr}}_{AC}[\rho^U_{BE|AC}(\rho_A \otimes \rho_C)]$ at E. Conversely, in case $C \rightarrow E$, then at least for some state ρ_A, if 'wiggling on C' by choosing different states ρ_C, then the marginal state ρ_E at E will 'wiggle', too. This is the essence of an interventionist account of causation that Secs. 3.2.2 and 3.2.4 touched on.

Suppose the channel $\rho_{BE|AC}$ describes a situation in which two agents have access to and can control systems A and C, respectively, and, possibly other agents, at a later time receive systems B and E. Also suppose that this channel arises from the unitary channel $\rho^U_{BEF|ACD}$ via $\rho_{BE|AC} = \overline{\text{Tr}}_D\text{Tr}_F[\rho^U_{BEF|ACD}\ \rho_D]$ for some state ρ_D and where D and F could be thought of as some respective environments. The unitary U has a causal structure according to Def. 4.3. As one would expect, if the respective agents can signal from C to E then the underlying unitary evolution U necessarily will be such that C is a direct cause of E. Suppose also A is a direct cause of E. Now it may however be the case that for the particular state ρ_D, for which the given channel $\rho_{BE|AC}$ arises, the possibility to signal from A to E disappears.

The approach taken here is based on taking quantum evolution to be fundamentally unitary, while non-unitary channels serve an effective description. Causal relations pertain to unitary transformations. As such, they are independent from agents, who might in principle be unable to access and control the system D in the above example to 'tune' the state ρ_D in such a way, so as to leverage the causal mechanism present in U to enable signalling from A to E.

On a second note, recall the remark from Sec. 3.2.4 that defining causation as signalling (relative to a generic channel) leads to an oddity. Given a channel $\rho_{B_1...B_k|A_1....A_n}$, it is generally not true that it satisfies an analogous property to that in Eq. (4.6) for no-signalling relations, that is, even if A_i cannot signal to B_j and also not to B_m, it may still be the case that it can signal to the composite system B_jB_m. While the overall causal structure of a unitary transformation is completely specified by the 'single-system' no-influence conditions — hence the terminology as in Def. 4.3 is justified — the overall signalling structure of a channel is not determined by the 'single-system' no-signalling conditions and is therefore not representable by a DAG.

As pointed out in Sec. 3.2.4, if one defined causal structure as a property of a generic channel given by the signalling relations, then causal structure would inherit that feature, making it incompatible with the idea that the presence and absence of a direct cause relation as encoded in a DAG can be considered individually.

4.2 Causal structure of unitary processes

In order to develop a framework of quantum causal models that rests on the above definition of quantum causal relations, it is necessary to spell out what that notion becomes at the level of quantum processes. This section will take that step and present the most general definition of causal structure aligned with that from Sec. 4.1. Substantiating that definition with intuition and discussing special cases is what the following chapters are reserved for.

Recall from Sec. 3.2.3 that any process $\sigma_{A_1 \ldots A_n}$ over the quantum nodes $A_1, \ldots, A_n$ defines a channel $\mathcal{P} : \mathcal{L}(\mathcal{H}_{A_1^{\text{out}}} \otimes \ldots \otimes \mathcal{H}_{A_n^{\text{out}}}) \to \mathcal{L}(\mathcal{H}_{A_1^{\text{in}}} \otimes \ldots \otimes \mathcal{H}_{A_n^{\text{in}}})$ from the output spaces of all nodes to their input spaces, with its CJ representation given by the process operator, $\sigma_{A_1 \ldots A_n} = \rho^{\mathcal{P}}_{A_1 \ldots A_n | A_1 \ldots A_n}$. Now, this channel may be a unitary channel.

Definition 4.4 (Unitary process): *A process $\sigma_{A_1 \ldots A_n}$ is called a unitary process if and only if its induced channel is a unitary channel, i.e. $\sigma_{A_1 \ldots A_n} = \rho^{U}_{A_1 \ldots A_1 | A_1 \ldots A_n}$.*

Note that the quantum nodes $A_1, \ldots, A_n$ are arbitrary quantum nodes, where some of the input and output spaces of the nodes may be trivial. The notion of no-influence from Def. 3.9 for unitary transformations then straightforwardly lifts to the notion of no-influence between the *quantum nodes* of a unitary process.

Definition 4.5 (No-influence in unitary process): *Given a unitary process $\sigma_{A_1 \ldots A_n} = \rho^{U}_{A_1 \ldots A_1 | A_1 \ldots A_n}$, write $A_j \nrightarrow A_i$, say 'node A_j* does not influence *node A_i', if and only if $A_j^{out} \nrightarrow A_i^{in}$ in U.*

Hence, stating the no-influence relations between the quantum nodes of a unitary process is a different way of stating the no-influence relations satisfied by the unitary transformation that is defined by the process. This difference in bookkeeping captures the fact that which pairs of spaces of a unitary transformation U — pairs of input and output to U — are taken to constitute a quantum node — the output and input of that node — plays a crucial role in the *causal* analysis of the matter of affairs. It also allows us to talk about quantum nodes as causal relata in a precise way. The analogues of Defs. 4.1 -4.3 in terms of nodes of unitary processes are then as follows.

Definition 4.6 (Direct cause relation and causal parents in unitary process): *Given a unitary process* $\sigma_{A_1...A_n} = \rho^U_{A_1...A_1|A_1...A_n}$, *node* A_j *is said to be a* direct cause *of node* A_i, *written* $A_j \to A_i$, *if and only if* A_j *can influence* A_i, *i.e.* $\neg(A_j \nrightarrow A_i)$. *For* $i \in \{1, ..., n\}$ *the set* $Pa(A_i) := \{A_j \mid j \in \{1, ..., n\}, A_j \to A_i\}$ *is called the* causal parents *of node* A_i.

Definition 4.7 (Causal structure of a unitary process): *Given a unitary process* $\sigma_{A_1...A_n} = \rho^U_{A_1...A_1|A_1...A_n}$, *the family of causal parents* $\{Pa(A_i)\}_{i=1}^n$ *is called its* causal structure *and can be represented by a directed graph with vertices* $A_1, ..., A_n$ *and an arrow from* A_j *to* A_i *whenever* $A_j \in Pa(A_i)$.

It follows from the property of unitary transformations (see Thm. 4.1 and subsequent discussion) that the causal structure of a unitary process, as defined in Def. 4.7, fully captures the direct-cause relations between its nodes — node A_i is a direct cause of the (composite) node defined by the pair A_j, A_m, if and only if it is a direct cause of at least one of them. Also note that due to unitarity, a node A_i is a root node in the causal structure of a unitary process if and only if A_i^{in} is a trivial space, and similarly, A_j is a leaf node if and only if A_j^{out} is a trivial space.

The causal structure of a unitary process represented as a directed graph G can be seen to arise from the DAG representing the causal structure of the associated unitary transformation, according to Def. 4.3, through merging the vertices corresponding to A_i^{in} and A_i^{out} into one vertex A_i for each $i = 1, \ldots, n$, while keeping all arrows. This may lead to directed cycles in the causal structure of a unitary process. The next chapter on quantum causal models will be exclusively concerned with the acyclic case, exploring this approach for when the causal structure is an 'ordinary' DAG. It is then Chap. 7 that is devoted to the study of when this is not the case.

Causal relata: arbitrary quantum nodes vs. quantum inodes

In above Def. 4.7, causal structure is defined as a property of any unitary process over arbitrary quantum nodes, which suggests that causal relata at a process level can be considered to be arbitrary quantum nodes. In contrast, Ref. [4] (see Sec. 3.2.5) and in fact our own work in Ref. [1] only considers quantum *i*nodes as causal relata (see Def. 3.11). There are good reasons for such restriction to quantum *i*nodes as explained in Sec. 3.2.5. Above all, it ensures that there always is the possibility to consider 'no intervention' at each node so as to view a quantum node as a representation of a quantum system, rather than necessarily as a locus of intervention. This is aligned with a programme that seeks to leave the role of agents reserved for studying causal relations but the latter itself can be defined as properties of underlying unitary evolution without agent-based terms.

The guiding attitude in this thesis will be the following. The notion of causal structure of a unitary process over general quantum nodes is a sound concept and leads to a formally more general framework. Seeing as the aspiration is to formulate the most general framework for causal reasoning, a restriction to quantum $i$nodes will *not* be imposed manifestly, except for in Secs. 5.3-5.6, where this is well-motivated and will be pointed out explicitly. Anything that follows, however, could be presented with a general restriction to quantum $i$nodes and one may think of this as a possible and intriguing perspective.

4.3 Causal relations and commutation relations

A central place in this thesis is taken by Thm. 4.1: the factorisation property of the CJ operator of a unitary channel, $\rho^U_{B_1\ldots B_k|A_1\ldots.A_n}$, into pairwise commuting marginal channels $\rho_{B_j|Pa(B_j)}$, as a consequence of the causal constraints U satisfies. It was already used to argue that the causal structure of a unitary transformation can indeed by represented by a DAG, as formalised in Def. 4.3. A noteworthy feature of the factorisation is that distinct factors $\rho_{B_j|Pa(B_j)}$ and $\rho_{B_m|Pa(B_m)}$ commute, while they both act non-trivially on the common causal parents $Pa(B_j) \cap Pa(B_m)$, which is in general a non-empty set. This has consequences concerning the algebraic structure of the Hilbert spaces, on which the operators act — a decomposition of the space associated with $Pa(B_j) \cap Pa(B_m)$, which lets one understand the conjunction of commutation and non-trivial action on that space. The following lemma states this decomposition.

Lemma 4.1 ([4]): *Let $\rho_{A|CD}$ and $\rho_{B|DE}$ be CJ representations of channels. If they commute $[\rho_{A|CD}\ ,\ \rho_{B|DE}] = 0$, then there exists a decomposition of the Hilbert space on which the domains of the channels overlap, here denoted as D, into orthogonal subspaces*

$$\mathcal{H}_D = \bigoplus_i \mathcal{H}_{D_i^L} \otimes \mathcal{H}_{D_i^R}, \tag{4.7}$$

and families of channels $\{\rho_{A|CD_i^L}\}_i$ and $\{\rho_{B|D_i^R E}\}_i$, such that

$$\rho_{A|CD} = \bigoplus_i \rho_{A|CD_i^L} \otimes \mathbb{1}_{(D_i^R)^*} \tag{4.8}$$

$$\rho_{B|DE} = \bigoplus_i \mathbb{1}_{(D_i^L)^*} \otimes \rho_{B|D_i^R E}\ . \tag{4.9}$$

Remark 4.1 *As is common, it will be useful at times to write* $\sum_i \rho_{A|CD_i^L} \otimes \mathbb{1}_{(D_i^R)^*}$, *where the summands are regarded as operators on the whole Hilbert space and act as zero maps on all but the* i*th subspace.*

Proof of Lem. 4.1. Ignoring negligible details the below proof already appeared in Ref. [4], but is restated here for the sake of completeness. Consider the channel $\rho_{AB|CDE} := \rho_{A|CD}\rho_{B|DE}$. One can directly verify that, as a consequence of the commuting factors, the quantum conditional mutual information $I(AC : BE|D)$ vanishes, if evaluated on the trace-1 quantum state $\hat{\rho}_{AB|CDE} = (1/(d_C d_D d_E))\rho_{AB|CDE}$. Theorem 6 of Ref. [122] then implies that there exists a decomposition of $\mathcal{H}_D$ into orthogonal subspaces of the form of Eq. (4.7), along with a probability distribution $\{p_i\}$, such that

$$\hat{\rho}_{AB|CDE} = \sum_i p_i \big(\hat{\rho}_{A|CD_i^L} \otimes \hat{\rho}_{B|D_i^R E}\big) , \tag{4.10}$$

where $\hat{\rho}_{A|CD_i^L}$ and $\hat{\rho}_{B|D_i^R E}$ are (trace-1) quantum states on the indicated Hilbert spaces. The normalization condition for the CJ representation of a channel, $\mathrm{Tr}_{AB}[\rho_{AB|CDE}] = \mathbb{1}_{(CDE)^*}$, fixes the p_i such that

$$\rho_{AB|CDE} = \sum_i \big[\ \rho_{A|CD_i^L} \otimes \rho_{B|D_i^R E}\ \big] , \tag{4.11}$$

where now each operator on the RHS is normalized as CJ operator of a channel, that is for each i, $\mathrm{Tr}_A[\rho_{A|CD_i^L}] = \mathbb{1}_{(CD_i^L)^*}$, and $\mathrm{Tr}_B[\rho_{B|D_i^R E}] = \mathbb{1}_{(D_i^R E)^*}$. The orthogonality of the subspaces means that the marginals $\rho_{A|CD}$ and $\rho_{B|DE}$ can indeed be written as claimed in Eqs. (4.8)-(4.9). □

Remark 4.2 *Strictly speaking, there is in general no equivalence between* $\mathcal{H}_D$ *and* $\bigoplus_i \mathcal{H}_{D_i^L} \otimes \mathcal{H}_{D_i^R}$ *— it is only an equivalence up to a unitary isomorphism. As is common practice, the presentation of Lem. 4.1 leaves this implicit for better readibility. However, in Chap. 6, since useful there, a statement of Lem. 4.1 will be given that makes explicit the unitary map, which 'identifies the decomposition'.*

Lemma 4.1 will be a recurring tool for proving results throughout the following chapters. The further study of the link between causal and compositional structure as such will be the very content of Chap. 6.

Chapter 5

The framework of quantum causal models

Section 3.2 argued why it is crucial to establish a framework of quantum causal models and summarised how prior work paved the way. This chapter, which is largely based on the first publication in Ref. [1], presents a fully-fledged framework based on the definition from Ref. [4]. It first states the definition of quantum causal models, which is then rooted in the notion of quantum causal structure from Chapter 4. The remainder of the chapter explores the framework and proves quantum generalisations of main theorems of the classical framework from Sec. 3.1.

5.1 The definition

The definition of this chapter's central object of study — a *quantum causal model* — is restated here for the sake of completeness, as well as, for a slight generalisation compared to the original Def. 3.12 from Ref. [4], by allowing arbitrary quantum nodes.

Definition 5.1 (Quantum causal model): *A* Quantum causal model *(QCM) is given by:*

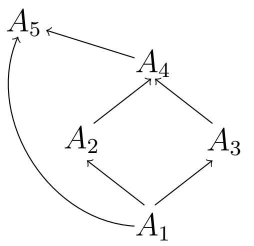
(1) *a causal structure represented by a DAG G with vertices corresponding to quantum nodes $A_1, ..., A_n$,*

(2) *for each A_i, a quantum channel $\rho_{A_i|Pa(A_i)} \in \mathcal{L}(\mathcal{H}_{A_i^{in}} \otimes \mathcal{H}^*_{Pa(A_i)^{out}})$ such that for all i, j, $[\rho_{A_i|Pa(A_i)}\ ,\ \rho_{A_j|Pa(A_j)}] = 0$.*

It defines a process operator over the quantum nodes $A_1, ..., A_n$ given by

$$\sigma_{A_1...A_n} = \prod_i \rho_{A_i|Pa(A_i)}\ . \tag{5.1}$$

See Fig. 5.1 for a generic example of a QCM.



$$\sigma_{A_1A_2A_3A_4A_5} = \rho_{A_5|A_1A_4}\ \rho_{A_4|A_2A_3}\ \rho_{A_2|A_1}\ \rho_{A_3|A_1}\ \rho_{A_1}$$

Figure 5.1: A quantum causal model.

Remark 5.1 *Suppose $A_1, \ldots, A_n$ are quantum nodes and $\{Pa(A_i)\}_i$ are the parental sets of a DAG with vertices $A_1, \ldots, A_n$. The fact that then any product of pairwise commuting operators of the form $\prod_i \rho_{A_i|Pa(A_i)}$ defines a process operator, as claimed in Def. 5.1, is straightforward due to the commutativity. There exists a total order of the nodes (let this be $A_1, \ldots, A_n$) such that $A_i \notin Pa(A_j)$ for any $i \geq j$. Hence, for any choice of CPTP maps at the n nodes $\{\tau_{A_i}\}_i$, it holds that*

$$\mathrm{Tr}_{A_1\ldots A_n}\Big[\prod_{i=1}^{n} \rho_{A_i|Pa(A_i)}\ \tau_{A_i}\Big] = \mathrm{Tr}_{A_1\ldots A_{n-1}}\Big[\Big(\prod_{i=1}^{n-1} \rho_{A_i|Pa(A_i)}\tau_{A_i}\Big)\mathrm{Tr}_{A_n}\big[\rho_{A_n|Pa(A_n)}\tau_{A_n}\big]\Big]$$
$$= \mathrm{Tr}_{A_1\ldots A_{n-1}}\Big[\prod_{i=1}^{n-1} \rho_{A_i|Pa(A_i)}\tau_{A_i}\Big] = \ldots = 1 .$$

Thus, by Def. 3.7, $\prod_i \rho_{A_i|Pa(A_i)}$ is a process operator. It is also immediate that it is a quantum $(n+1)$-comb, as defined in Ref. [32], for the same total order of nodes $A_1, \ldots, A_n$ (see Sec. 3.2.3).

The reason for allowing arbitrary quantum nodes as causal relata in Def. 5.1, despite the main intended usage of the framework as one for causal reasoning about quantum *i*nodes (see Def. 3.11), was explained in Sec. 4.2. It is useful to give the constraint from causal structure, expressed in the quantum causal principle (Principle 2), only now allowing arbitrary quantum nodes, a name.

Definition 5.2 (Quantum Markov condition): *Given a DAG G, with vertices corresponding to the quantum nodes $A_1, \ldots, A_n$, a process $\sigma_{A_1\ldots A_n}$ is called* Markov *for G if and only if it admits a factorization into pairwise commuting channels of the form $\sigma_{A_1\ldots A_n} = \prod_{i=1}^{n} \rho_{A_i|Pa(A_i)}$.*

This generalises the classical notion of Markovianity (cf. Def. 3.2) to the quantum case[1] and allows reference to the data of a QCM as a pair $(G, \sigma_{A_1\ldots A_n})$, where G is

[1]See Sec. 5.3 for a detailed analysis of how the former is a special case of the latter.

a DAG with vertices $A_1, \dots, A_n$ and $\sigma_{A_1 \dots A_n}$ a process that is Markov for G.

It also generalises the definition of the quantum Markov condition from Ref. [82] that was already mentioned in Sec. 3.2.4. According to that notion, each output system A_i^{out} factorises into as many subsystems as the vertex A_i has children, i.e. A_i^{out} has subsystems $A_i^{(j)}$ for all j such that $A_j \in Ch(A_i)$. The CJ operator $\rho_{A_j|Pa(A_j)}$ is then assumed to represent a channel of the form $\mathcal{L}(\bigotimes_{A_i \in Pa(A_j)} \mathcal{H}_{A_i^{(j)}}) \rightarrow \mathcal{L}(\mathcal{H}_{A_j^{in}})$. Hence, as far as the parent node A_i is concerned, the operator $\rho_{A_j|Pa(A_j)}$ acts non-trivially only on the $A_i^{(j)}$ subsystem. The pairwise commutation of all the operators $\rho_{A_i|Pa(A_i)}$ therefore becomes trivial, despite the generally overlapping parental sets. The physical intuition behind the Markov condition from Ref. [82] is clear: a physical system — the respective subsystem $A_i^{(j)}$ — can be thought to 'travel' from A_i to A_j, thereby mediating the asserted causal mechanism (see Sec. 3.2.4).

However, this is not the most general condition to warrant a corresponding causal explanation of all those cases, where we have a good understanding of what the causal explanation should be, as argued in Ref. [4] (see Sec. 3.2.5). But what then justifies the general quantum causal principle, that is, why should Markovianity for a DAG G according to Def. 5.2, be the correct necessary condition for regarding G as a plausible causal structure of the involved nodes? The next section offers an answer to this question.

5.2 Causal structure and the Markov condition

This section presents one of the main results — the last missing piece in the quantum analogue of the blueprint from Sec. 3.1.2: a generalisation to arbitrary DAGs of Thm. 3.4 that concerns the quantum complete common cause scenario, and simultaneously, a generalisation from classical to quantum of Thm. 3.1, that concerns arbitrary DAGs. We start by developing the necessary terms.

5.2.1 Compatibility with causal structure

Let us forget about the proposed quantum causal models for a moment. Chapter 4 defined what it means for a node A_j to be a direct cause of node A_i given a *unitary* process $\sigma_{A_1 \dots A_n}$ (cf. Def. 4.6) and what the causal structure of a unitary process is (cf. Def. 4.7).

Now, given a *non-unitary* process $\sigma_{A_1 \dots A_n}$, the idea is that there always is an underlying unitary process and it is that which the causal structure is a property of. Suppose this causal structure is a DAG, recalling that in this chapter we restrict our attention to *acyclic* causal structures. More concretely, suppose

$\sigma_{A_1 \ldots A_n} = \mathrm{Tr}_{FP}[\sigma_{A_1 \ldots A_n FP}\ \tau_P]$ for some state $\tau_P \in \mathcal{L}(\mathcal{H}^*_{P^{\mathrm{out}}})$ and some unitary process $\sigma_{A_1 \ldots A_n FP} = \rho^U_{A_1 \ldots A_n F | A_1 \ldots A_n P}$ with root node P and leaf node F and the DAG G as its causal structure of the $n+2$ nodes. What is the status of the subgraph G' defined by ignoring the vertices F and P as well as any arrows involving these two nodes? Is this *the* causal structure of the nodes $A_1, \ldots, A_n$? If P is a common cause of at least two distinct nodes A_i and A_k, the answer ought to be 'no', for it would be an incomplete causal characterisation of the nodes $A_1, \ldots, A_n$. This is in analogy to how, classically, common causes in general underwrite correlations that can only be made sense of in light of all common causes. If in turn the restriction to a subgraph G' by ignoring some nodes and all arrows involving those nodes, does not omit any common causes to the nodes in G', then these remaining nodes may be regarded as a *causally complete* set of nodes. It is thus natural to call a process $\sigma_{A_1 \ldots A_n}$ compatible with a DAG G if it is possible to see $\sigma_{A_1 \ldots A_n}$ as arising from a unitary process with a corresponding causal structure, without having to introduce further common causes. More formally, and generalising Def. 3.10:[2]

Definition 5.3 (Compatibility with DAG): *A process $\sigma_{A_1 \ldots A_n}$ is* compatible *with a DAG G with vertices $A_1, ..., A_n$, if and only if a unitary process $\sigma_{A_1 \ldots A_n \lambda_1 \ldots \lambda_n F} = \rho^U_{A_1 \ldots A_n F | A_1 \ldots A_n \lambda_1 \ldots \lambda_n}$ exists, with an extra root node λ_i for $i = 1, ..., n$ and an extra leaf node F, such that:*

(1) *the process $\sigma_{A_1 \ldots A_n}$ is recovered as the marginal process on nodes $A_1, \ldots, A_n$ for some product state $\tau_{\lambda_1} \otimes \cdots \otimes \tau_{\lambda_n}$ with $\tau_{\lambda_i} \in \mathcal{L}(\mathcal{H}^*_{\lambda_i^{out}})$, i.e.*

$$\sigma_{A_1 \ldots A_n} = \mathrm{Tr}_{F \lambda_1 \ldots \lambda_n} \left[\, \sigma_{A_1 \ldots A_n \lambda_1 \ldots \lambda_n F}\ (\tau_{\lambda_1} \otimes \cdots \otimes \tau_{\lambda_n}) \right] \ , \tag{5.2}$$

(2) *the unitary process $\sigma_{A_1 \ldots A_n \lambda_1 \ldots \lambda_n F}$ satisfies the following causal constraints (with $Pa(A_i)$ referring to G):*

$$\{A_j \nrightarrow A_i\}_{A_j \notin Pa(A_i)} \ , \ \{\lambda_j \nrightarrow A_i\}_{j \neq i} \, . \tag{5.3}$$

Note that compatibility with a DAG G through Eq.(5.3) only requires that the asserted underlying unitary process satisfies the no-influence conditions that are encoded in G through absences of arrows. It does not require that these are the only ones, i.e. that all arrows in G actually correspond to the presence of influence in that unitary process. This is aligned with a tradition in classical causal modeling in that

[2]Note that if a process is compatible with a DAG, it is in particular 'unitarily extendible', a concept, which was first introduced in Ref. [123] under the name of 'purifiability', and which will be defined and studied in Chap. 7.

it is the absences of causal relations which impose constraints, and it is those that the underlying unitary process has to respect at the very least. Def. 5.3 thus captures the minimum requirements for a notion of compatibility, while a conceivable stronger notion would require that all arrows in G correspond to direct-cause relations in the underlying unitary process. (Also see discussions in Secs. 5.2.3 and 5.7.)

5.2.2 Compatibility and unitary circuits

The above argued why the notion of compatibility with a DAG captures what its name suggests. However, the unitary processes thereby asserted to exist are abstract objects. At the same time, in the 'acyclic regime' where causal structure can be represented with a DAG, we have a clear intuition for how quantum systems evolve, namely, in a fashion that is representable with quantum circuits.

In order to see how a unitary circuit can induce a unitary process, the concept of a *broken unitary circuit* is helpful. Suppose a unitary circuit is given as in Fig. 5.2a, and suppose that then at the places A_1, A_2, A_3 and A_4 the wires are 'broken', creating four slots that define the respective quantum $\imath$nodes A_1, A_2, A_3 and A_4, where for each $i = 1, ..., 4$ the respective bottom open wire, 'going into' A_i, represents the space $\mathcal{H}_{A_i^{\text{in}}}$ and the top open wire, 'coming out' of A_i, represents the space $\mathcal{H}_{A_i^{\text{out}}}$. This defines the unitary map $U : \left(\bigotimes_{j=1}^{3} \mathcal{H}_{R_j}\right) \otimes \left(\bigotimes_{i=1}^{4} \mathcal{H}_{A_i^{\text{out}}}\right) \rightarrow \left(\bigotimes_{m=1}^{3} \mathcal{H}_{L_m}\right) \otimes \left(\bigotimes_{i=1}^{4} \mathcal{H}_{A_i^{\text{in}}}\right)$. That this map U in turn defines a unitary process with root nodes R_1, R_2, R_3, leaf nodes L_1, L_2, L_3 and $\imath$nodes $A_1, \ldots, A_4$ is evident from its circuit structure: no matter which CPTP maps are inserted into $A_1, \ldots, A_4$ and which states fed into R_1, R_2, R_3, tracing L_1, L_2, L_3 always yields the real number 1. Similarly, given any unitary circuit, letting the originally open ingoing and outgoing wires define root and leaf nodes, respectively, and if an arbitrary number of wires is 'broken' to define further $\imath$nodes, this defines a broken unitary circuit.

As a unitary process, a broken unitary circuit has a DAG as causal structure. The causal structure of the one from Fig. 5.2b will in general be a subgraph of the DAG in Fig. 5.2c, since the component unitaries themselves and their composition as in Fig. 5.2b might satisfy further causal constraints not evident from the circuit (also see Chap. 6). If causal relata are considered to be quantum $\imath$nodes, a broken unitary circuit with a causal structure that respects the corresponding causal constraints from Def. 5.3 is just what one would expect to exist in case a process is compatible with some DAG. The broken unitary circuit describes how the quantum systems evolve, where the broken wires of the circuit allow us to reason about what would be the case, were one to consider an external intervention on the respective system, even though it is otherwise just an ordinary quantum circuit.

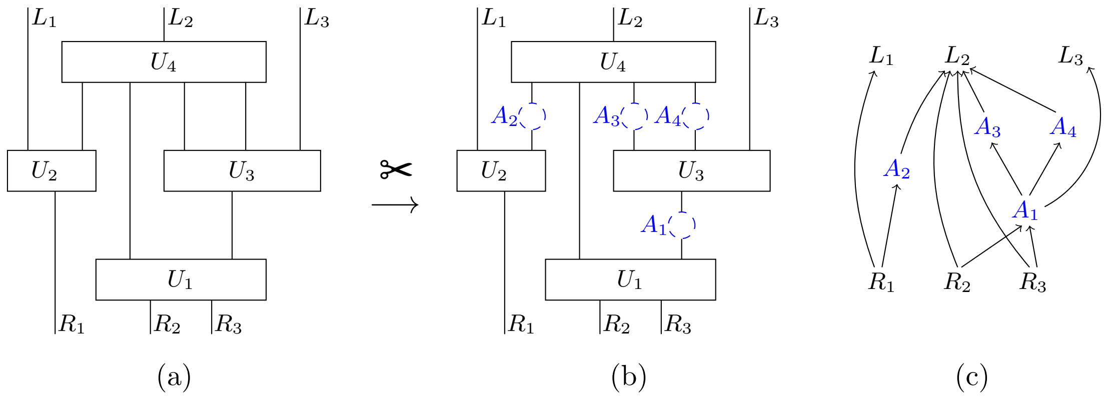


Figure 5.2: Example of a *broken unitary circuit* in (b), which can be seen to arise from the circuit in (a), and in (c) the DAG that encodes all no-influence conditions as manifest from (b) [30].

In the general framework the quantum nodes of a process that is compatible with some DAG may be arbitrary. In order to see how a unitary process that involves such general nodes, can arise from a unitary circuit, consider again the same example of a unitary circuit, reproduced in Fig. 5.3a. This time, once some wires are broken, rather than necessarily taking the 'slot' of a single broken wire to define a quantum node, instead let the quantum node be defined by the gap created from taking a whole unitary circuit fragment out, as illustrated in the example in Fig. 5.3.

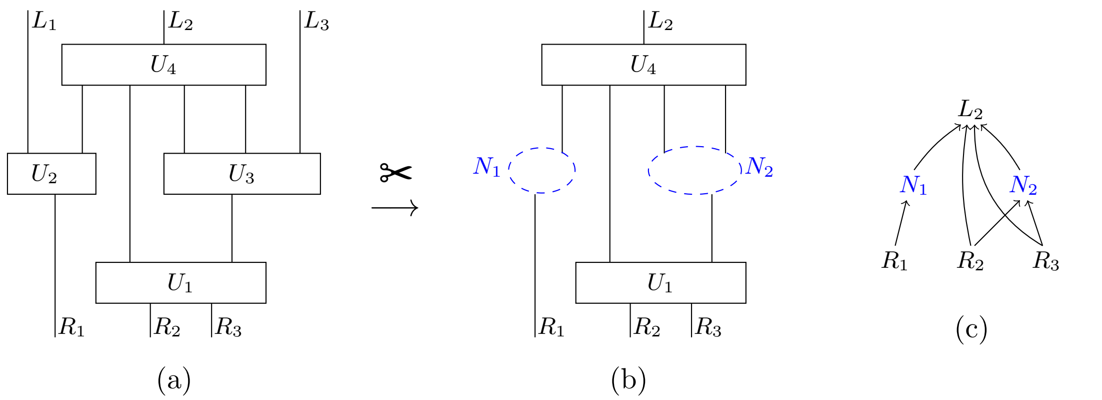


Figure 5.3: Example of a *broken unitary circuit* in (b), which can be seen to arise from the circuit in (a) by taking circuit fragments out, and in (c) the DAG that encodes all no-influence conditions as manifest from (b) [30].

The general object that can arise in such a way, that is, as a composition of unitary circuit fragments, where some sets of open wires are taken to define quantum nodes, will still be referred to as a broken unitary circuit. The following theorem then fills the gap and brings the intuition of unitary circuits to the notion of compatibility.

Theorem 5.1 *Consider a DAG G with nodes $A_1, \ldots, A_n$, labelled such that the total order $A_1 < \cdots < A_n$ is compatible with the partial order defined by G. Suppose that a process $\sigma_{A_1 \ldots A_n}$ is compatible with G. Let $\sigma_{A_1 \ldots A_n \lambda_1 \ldots \lambda_n F} = \rho^U_{A_1 \ldots A_n F | A_1 \ldots A_n \lambda_1 \ldots \lambda_n}$ be the unitary process, whose existence is asserted by the definition of compatibility, that is, satisfies Eq.5.2 for some product state $\tau_{\lambda_1} \otimes \cdots \otimes \tau_{\lambda_n}$ and also satisfies the causal constraints from Eq.* (5.3). *Then there exists a* broken unitary circuit *of the form of Fig. 5.4 that is a* realization *of $\sigma_{A_1 \ldots A_n \lambda_1 \ldots \lambda_n F}$, i.e.,*

$$\sigma_{A_1 \ldots A_n \lambda_1 \ldots \lambda_n F} \;=\; \overline{\mathrm{Tr}}_{A'_1 \ldots A'_n} \left[\rho^{U_{n+1}}_{F|A_n A'_n} \left(\prod_{i=2}^{n} \rho^{U_i}_{A_i A'_i | A_{i-1} A'_{i-1} \lambda_i} \right) \rho^{U_1}_{A_1 A'_1 | \lambda_1} \right] . \tag{5.4}$$

Proof. See App. A.2. ☐

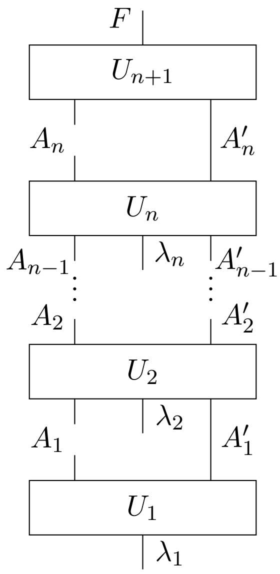


Figure 5.4: A broken unitary circuit as implied to exist by compatibility of a process with a DAG.

Note that in Eq. (5.4) the intermediate primed systems A'_i are ordinary quantum systems, while the A_i are quantum nodes and hence, following our convention for suppressing 'in' and 'out' for the respective spaces in CJ operators (see Sec. 3.2.3), the ith unitary is of the form $U_i \;:\; \mathcal{H}_{A^{\text{out}}_{i-1}} \otimes \mathcal{H}_{A'_{i-1}} \otimes \mathcal{H}_{\lambda_i} \;\to\; \mathcal{H}_{A^{\text{in}}_i} \otimes \mathcal{H}_{A'_i}$.

The unitary process asserted to exist by compatibility with a DAG G is by definition a *unitary quantum comb*, that is, a unitary process which also is a quantum comb as originally defined in Ref. [32] (see Sec. 3.2.3). As such, Ref. [32] showed it to always have a realisation as a *quantum network* of a similar form as in Fig. 5.4, but with isometries as the component maps, where Fig. 5.4 shows the unitary maps U_i. Dilating these isometries to unitary maps will in general require further auxiliary input systems, which cannot (at least not in an obvious way) be guaranteed to not be additional common causes to some of the quantum nodes. That, however, is the core of the notion of compatibility, hence, the need of Thm. 5.1. Note that in the proof in App. A.2 it is an iterative use of Lem. 4.1 that essentially reveals the decomposition of the unitary transformation U into the component unitaries U_i.

5.2.3 Equivalence Markovianity and compatibility

Theorem 5.2 *Given a DAG G with nodes $A_1, \ldots, A_n$, and a process $\sigma_{A_1 \ldots A_n}$, the following are equivalent:*

(1) $\sigma_{A_1 \ldots A_n}$ *is compatible with G.*

(2) $\sigma_{A_1 \ldots A_n}$ *is Markov for G.*

Proof: (1) $\rightarrow$ (2)**.** Suppose $\sigma_{A_1 \ldots A_n}$ is compatible with G and let $\sigma_{A_1 \ldots A_n \lambda_1 \ldots \lambda_n F} = \rho^U_{A_1 \ldots A_n F | A_1 \ldots A_n \lambda_1 \ldots \lambda_n}$ be the unitary process asserted to exist by assumption of compatibility with G. Let $Pa(A_i)$ denote the parental sets of the nodes A_i according to the DAG G. Due to the no-influence conditions specified in Eq. 5.3, the causal parents of A_i in the unitary U then have to be contained in $Pa(A_i) \cup \{\lambda_i\}$ and hence, by Thm. 4.1, it holds that

$$\rho^U_{A_1 \ldots A_n F | A_1 \ldots A_n \lambda_1 \ldots \lambda_n} = \rho_{F | A_1 \ldots A_n \lambda_1 \ldots \lambda_n} \left(\prod_i \rho_{A_i | Pa(A_i) \lambda_i} \right) . \tag{5.5}$$

Marginalizing over F and the λ_i for the appropriate states $\tau_{\lambda_i} \in \mathcal{L}(\mathcal{H}^*_{\lambda_i^{\text{out}}})$, also asserted to exist by assumption of compatibility, gives

$$\begin{aligned} \sigma_{A_1 \ldots A_n} &= \mathrm{Tr}_{F \lambda_1 \ldots \lambda_n} \Big[\rho^U_{A_1 \ldots A_n F | A_1 \ldots A_n \lambda_1 \ldots \lambda_n} \left(\tau_{\lambda_1} \otimes \cdots \otimes \tau_{\lambda_n} \right) \Big] \\ &= \mathrm{Tr}_F \big[\rho_{F | A_1 \ldots A_n \lambda_1 \ldots \lambda_n} \big] \left(\prod_i \mathrm{Tr}_{\lambda_i} \big[\rho_{A_i | Pa(A_i) \lambda_i} \, \tau_{\lambda_i} \big] \right) \quad (5.6) \\ &= \prod_i \rho_{A_i | Pa(A_i)} , \quad (5.7) \end{aligned}$$

where $\rho_{A_i|Pa(A_i)} := \mathrm{Tr}_{\lambda_i} \big[\rho_{A_i | Pa(A_i) \lambda_i} \, \tau_{\lambda_i} \big]$ and $[\rho_{A_i|Pa(A_i)} \, , \, \rho_{A_j|Pa(A_j)}] = 0$ for all i, j, since $[\rho_{A_i|Pa(A_i)\lambda_i} \, , \, \rho_{A_j|Pa(A_j)\lambda_j}] = 0$ for all i, j. Hence $\sigma_{A_1 \ldots A_n}$ is Markov for G. $\square$

For the converse direction, (2) $\rightarrow$ (1), as well as, for many later proofs the following notion will be useful.

Definition 5.4 (Reduced unitary channel[3]): *A channel* $\mathcal{C} : \mathcal{L}(\mathcal{H}_A) \to \mathcal{L}(\mathcal{H}_B)$ *is a* reduced unitary channel *if and only if there exists a unitary transformation* $U : \mathcal{H}_A \to \mathcal{H}_B \otimes \mathcal{H}_F$ *such that* $\rho^{\mathcal{C}}_{B|A} = \mathrm{Tr}_F[\rho^U_{FB|A}]$.

Lemma 5.1 *Suppose* $\rho_{B|A}$ *and* $\rho_{C|A}$ *represent reduced unitary channels and satisfy* $[\rho_{B|A}\ ,\ \rho_{C|A}] = 0$. *Then the channel represented by their product* $\rho_{BC|A} := \rho_{B|A}\ \rho_{C|A}$ *is also a reduced unitary channel.*

Proof of Lem. 5.1. See App. A.3. □

Proof: (2) → (1) **of Thm. 5.2.** Suppose $\sigma_{A_1\ldots A_n}$ is Markov for G. For improved legibility of the following proof, write $P_i := Pa(A_i)$. By assumption, there exist pairwise commuting channels $\rho_{A_i|P_i}$, such that $\sigma_{A_1\ldots A_n} = \prod_i \rho_{A_i|P_i}$. In particular, $[\rho_{A_1|P_1}\ ,\ \rho_{\overline{A_1}|P_1\overline{P_1}}] = 0$, where $\overline{P_1} := \{A_1, \ldots, A_n\} \setminus P_1$, so that $\rho_{\overline{A_1}|P_1\overline{P_1}} = \prod_{i\neq 1} \rho_{A_i|P_i}$. Lem. 4.1 implies that there exists a decomposition of $\mathcal{H}_{P_1^{\text{out}}}$ into orthogonal subspaces $\mathcal{H}_{P_1^{\text{out}}} = \bigoplus_j\ \mathcal{H}_{(P_1)^L_j} \otimes \mathcal{H}_{(P_1)^R_j}$ such that

$$\rho_{A_1|P_1} \;=\; \sum_j \rho_{A_1|(P_1)^L_j} \otimes \mathbb{1}_{(P_1)^R_j}\ , \tag{5.8}$$

$$\rho_{\overline{A_1}|P_1\overline{P_1}} \;=\; \sum_j \mathbb{1}_{(P_1)^L_j} \otimes \rho_{\overline{A_1}|(P_1)^R_j\overline{P_1}}\ , \tag{5.9}$$

where on the right-hand sides the 'stars' indicating the action of the identity operators on the dual spaces have been suppressed to avoid clutter, and the ordinary sum symbols are in keeping with the convention from Rem. 4.1. For each j, the channel represented by $\rho_{A_1|(P_1)^L_j}$ can be dilated to a unitary channel with unitary $V_j : \mathcal{H}_{(P_1)^L_j} \otimes \mathcal{H}_{(\lambda_1)_j} \to \mathcal{H}_{A_1} \otimes \mathcal{H}_{F_j}$ and some appropriate state $|0\rangle_{(\lambda_1)_j}$. Let λ_1 be a system of large enough dimension such that these unitaries can be extended to $V_j : \mathcal{H}_{(P_1)^L_j} \otimes \mathcal{H}_{\lambda_1} \to \mathcal{H}_{A_1} \otimes \mathcal{H}_{F_j}$ (for appropriate F_j) with a common auxiliary state $|0\rangle_{\lambda_1}$. Define the unitary $V : \mathcal{H}_{P_1} \otimes \mathcal{H}_{\lambda_1} \to \mathcal{H}_{A_1} \otimes \mathcal{H}_F$ by setting $\mathcal{H}_F := \bigoplus_j \mathcal{H}_{F_j} \otimes \mathcal{H}_{(P_1)^R_j}$ and $V := \bigoplus_j V_j \otimes \mathbb{1}_{(P_1)^R_j}$. By construction,

$$\rho_{A_1|P_1} \;=\; \mathrm{Tr}_F\overline{\mathrm{Tr}}_{\lambda_1}\Big[\ \rho^V_{A_1F|P_1\lambda_1}\ \ |0\rangle_{\lambda_1}\langle 0|\ \Big]\ . \tag{5.10}$$

The marginal channel $\rho_{A_1|P_1\lambda_1} = \mathrm{Tr}_F[\rho^V_{A_1F|P_1\lambda_1}]$ is by definition a reduced unitary channel, and it commutes with $\rho_{A_j|P_j}$ for all $j \neq 1$. Next, consider $[\rho_{A_2|P_2}\ ,\ \rho_{\overline{A_2}|P_2\overline{P_2}\lambda_1}] = 0$, where $\rho_{\overline{A_2}|P_2\overline{P_2}\lambda_1} := \rho_{A_1|P_1\lambda_1}\big(\prod_{i=3}^n \rho_{A_i|P_i}\big)$. A similar construction to the above yields a corresponding channel $\rho_{A_2|P_2\lambda_2}$. Iterating this procedure yields a set of

[3] This terminology was first used in Ref. [1]. In Ref. [16], the same concept is called 'autonomy' of a channel.

pairwise commuting reduced unitary channels, $\{\rho_{A_i|P_i\lambda_i}\}$, such that for each i, the reduced unitary channel $\rho_{A_i|P_i\lambda_i}$ returns the original channel $\rho_{A_i|P_i}$ for some state ρ_{λ_i}. Lem. 5.1 then implies that $\prod_i \rho_{A_i|P_i\lambda_i}$ represents a reduced unitary channel, too, and hence, there exists a unitary U such that

$$\mathrm{Tr}_F\Big[\ \rho^U_{A_1...A_nF|A_1...A_n\lambda_1...\lambda_n}\ \Big] = \prod_i \rho_{A_i|P_i\lambda_i}\ . \tag{5.11}$$

By construction,

$$\sigma_{A_1...A_n} \ = \ \overline{\mathrm{Tr}}_{\lambda_1...\lambda_n}\mathrm{Tr}_F\Big[\ \rho^U_{A_1...A_nF|A_1...A_n\lambda_1...\lambda_n}\ (\rho_{\lambda_1}\otimes\cdots\otimes\rho_{\lambda_n})\ \Big], \tag{5.12}$$

and the unitary U satisfies the no-influence conditions:

$$\big\{A_j^{\mathrm{out}} \nrightarrow A_i^{\mathrm{in}}\big\}_{A_j\notin Pa(A_i)}\ ,\ \big\{\lambda_j \nrightarrow A_i^{\mathrm{in}}\big\}_{j\neq i} \quad \forall i=1,\ldots,n. \tag{5.13}$$

It is straightforward to see that this unitary channel defines a unitary process with the required properties. Let us formally see the systems λ_i as defining the output spaces of root nodes, also labelled λ_i, and similarly, F as defining the input space of a leaf node F. The states ρ_{λ_i} induce states $\tau_{\lambda_i} \in \mathcal{L}(\mathcal{H}^*_{\lambda_i^{\mathrm{out}}})$ such that Eq. (5.12) can be rewritten with traces over nodes $F\lambda_1...\lambda_n$ as in Eq.(5.2). Noting Rem. 5.1 it then follows that $\rho^U_{A_1...A_nF|A_1...A_n\lambda_1...\lambda_n}$ indeed defines a unitary process with, due to Eq. (5.13), the desired causal constraints as required by Def. 5.3. □

Note that the above proof of direction '(1) → (2)' also makes explicit how it follows immediately from Thm. 4.1 that any unitary process with an acyclic causal structure G defines a quantum causal model.

Finally, recall that Sec. 5.2.1 mentioned a conceivable, stronger notion of compatibility with a DAG G that demands that the underlying unitary process actually allows causal influences according to all arrows in G. Whether Thm. 5.2 can then be strengthened to an equivalence between Markovianity and such stronger notion of compatibility is an open question at the time of writing.

5.2.4 What the equivalence means for the framework

Sections 5.2.1 and 5.2.2 established that it is those processes that are compatible with a DAG G, for which G can be taken to be a plausible causal explanation. Thm. 5.2 establishes the equivalence between compatibility with a given DAG and Markovianity for that DAG. Thus it is the processes which are Markov for a DAG G that can be causally explained in terms of G.

Thm. 5.2 can therefore be seen to amount to a justification — at least a partial one — of the causal principle (Principle 3) and the definition of a quantum causal model. It is a justification on the grounds of two premises. First, causal relations are defined as influence in underlying unitary processes as in Sec. 4.2. Second, the notion of compatibility with a DAG G has built in that the given process $\sigma_{A_1...A_n}$ is obtained as the marginal process for a *product state* on the local disturbances λ_i. While the causal structure of the underlying unitary process is of course independent from which state is considered for $\lambda, \dots, \lambda_n$, the intuition behind requiring a product state is clear. Suppose $\sigma_{A_1...A_n}$ can be seen to arise from a unitary process that does not introduce further common causes to $A_1, ..., A_n$, however, that *requires a non-product state* for the systems λ_i. Then the latter fact is interpreted as a signature of that $\sigma_{A_1...A_n}$ contains 'correlations' between the systems λ_i, and that these λ_i can in fact *not* be regarded *local* disturbances, for they must have a common cause further down in the 'causal past', which leads to the necessity of a non-product state.

However, a justification of the product-state assumption that does not end up being circular, is beyond the scope of this work. Grounding this assumption in other, yet less ad-hoc premises may well not be independent from other deep questions, such as what the status and origin of an apparent arrow of time is and what the role of agents are. Note that it also is a common assumption in the classical literature to ascribe a product distribution accounting for the lack of knowledge over the local disturbances as mirrored in the classical case in Def. 3.4.

Note that also if not further justifying the product state assumption, a minimum consistency requirement for seeing Thm. 5.2 as a justification of the definition of a quantum causal model is 'Markov-stability': maintaining a product form, but changing which concrete state the systems λ_i are ascribed, should make no difference to the fact that the marginal process is Markov for G. Otherwise Markovianity could hardly be taken seriously as the condition that is the signature of having identified a plausible causal structure — the precise 'lack of knowledge' encoded in $\rho_{\lambda_1} \otimes \cdots \otimes \rho_{\lambda_n}$ had better stand apart from what the asserted causal structure is. It is immediate from Eq. (5.6) that this is the case. Markovianity is not an artifact from fine-tuning the local disturbances.

5.3 Relation quantum and classical causal models

This section will explain the relation between classical and quantum causal models, in particular, in what sense the former are special cases of the latter. To this end it introduces *classical split-node causal models*, which take an intermediate place between classical and quantum causal models and help to expose their relation. They will also be important for deriving and elucidating the results in Secs. 5.4-5.6.

Importantly, this section as well as the three subsequent ones — Secs. 5.4, 5.5 and 5.6 — will

only consider quantum $\imath$nodes

as the quantum nodes of quantum processes (see Def. 3.11). It will be understood implicitly that talking about quantum nodes refers to $\imath$nodes. Beyond dedicating these sections to the approach that takes causal relata to be quantum $\imath$nodes and the conceptual motivation behind that (see Sec. 4.2), the reason for this restriction also is that quantum nodes that are not $\imath$nodes, do not have an analogue in classical causal models. The following sections, however, develop quantum generalisations of core concepts and theorems of the classical framework, which either strictly require the restriction to quantum $\imath$nodes and or are strongly guided by the intuition in the classical case.

5.3.1 Classical process maps

The classical analogue of a quantum node is a *classical split node* X, given by a pair of classical variables of an input variable X^{in} and an output variable X^{out}, which are copies of each other. Completely analogous to the quantum case, the idea is that a classical split node constitutes a locus, where an intervention may take place. An *intervention at the classical split node* X with outcome k_X can be modeled by a classical instrument of the form $P(k_X, X^{\text{out}}|X^{\text{in}})$. If there is no outcome (i.e. trivial k_X), or equivalently, considering the effective intervention from marginalising over different outcomes, a corresponding intervention is given by a classical channel $P(X^{\text{out}}|X^{\text{in}})$. Particularly important is the representation of 'no intervention', namely as $P(X^{\text{out}}|X^{\text{in}}) = \delta(X^{\text{out}}, X^{\text{in}})$, analogous to the quantum case with τ_A^{id} at a quantum $\imath$node A. Also important and unique to the classical case is the concept of a perfect, non-disturbing measurement of the form $P(k_X, X^{\text{out}}|X^{\text{in}}) = \delta(X^{\text{out}}, X^{\text{in}})\delta(k_X, X^{\text{in}})$.

The classical analogue of a quantum process is a *classical process*, as defined in a corresponding framework to study the most general processes connecting a set of classical split nodes. This was introduced by Baumeler, Feix and Wolf in Ref. [47] and has been studied in detail in the literature[4] (see, e.g., Refs. [47, 52, 58, 69]). The main motivation behind these works, however, is to explore the conceivable classical

[4] Terminology tends to differ across different works, where e.g. in Ref. [47] split nodes are called 'local laboratories' and classical processes are called 'environments'.

processes which are incompatible with a definite causal order of the split nodes. A discussion of this purpose of the formalism and the seminal findings from these works will be postponed to Sec. 7.1.2. Here, the intention merely is to provide a general set-up for the formulation of classical causal models that is closer to the quantum framework and this chapter therefore focuses on scenarios, where a causal order of the split nodes exists.

A classical process can be represented by a classical process map:

Definition 5.5 (Classical process map): *A* classical process map *over classical split-nodes $X_1, ..., X_n$ is a map*

$$\kappa_{X_1 \ldots X_n} \ : \ X_1^{in} \times X_1^{out} \times \ldots \times X_n^{in} \times X_n^{out} \ \rightarrow \ [0,1] \ ,$$

such that for any set of classical channels $\{P(X_i^{out}|X_i^{in})\}$,

$$\sum_{X_1^{in}, X_1^{out}, \ldots, X_n^{in}, X_n^{out}} \left(\kappa_{X_1 \ldots X_n} \prod_i P(X_i^{out}|X_i^{in}) \right) \ = \ 1 \ . \tag{5.14}$$

Given a classical process map $\kappa_{X_1 \ldots X_n}$ and local interventions $P(k_{X_i}, X_i^{\text{out}}|X_i^{\text{in}})$ at the n nodes, the joint probability distribution over the outcomes is given by

$$P(k_{X_1}, ..., k_{X_n}) \ = \sum_{X_1^{\text{in}}, X_1^{\text{out}}, \ldots, X_n^{\text{in}}, X_n^{\text{out}}} \left(\kappa_{X_1 \ldots X_n} \prod_i P(k_{X_i}, X_i^{\text{out}}|X_i^{\text{in}}) \right), \tag{5.15}$$

where it follows from Def. 5.5 that the right-hand side indeed defines a correctly normalised probability distribution [47]. Note that it also follows from Eq. (5.14) that, analogously to the quantum case, a classical process map $\kappa_{X_1 \ldots X_n}$ defines a classical channel $P(X_1^{\text{in}}, \ldots, X_n^{\text{in}}|X_1^{\text{out}}, \ldots, X_n^{\text{out}})$ from the output variables at all nodes to the input variables at all nodes. However, just as with the quantum case, not all channels of the form $P(X_1^{\text{in}}, \ldots, X_n^{\text{in}}|X_1^{\text{out}}, \ldots, X_n^{\text{out}})$ define a classical process map.

In order to enable analogous notation to that for quantum processes (Sec. 3.2.3), the following are some useful conventions. A classical instrument $P(k_X, X^{\text{out}}|X^{\text{in}})$ will often be denoted as $\tau_X^{k_X}$, which, for each k_X, is seen as a map of the form $X^{\text{out}} \times X^{\text{in}} \rightarrow [0,1]$ (the context will always make it unambiguous, whether it is a classical or quantum instrument). In particular, write $\tau_X^{\text{id}} = \delta(X^{\text{out}}, X^{\text{in}})$ for the 'no intervention'. Otherwise an intervention without outcome (trivial k_X) is denoted τ_X. Analogously to Tr_A for a quantum node A we write $\sum_X$ as short-hand for $\sum_{X^{\text{in}}, X^{\text{out}}}$.

Concerning a set of split nodes $S = \{X_1, \ldots, X_n\}$, writing S^{in} stands for the tuple $(X_1^{\text{in}}, \ldots, X_n^{\text{in}})$, analogously for S^{out}, and $\sum_S$ is short for $\sum_{X_1,\ldots,X_n}$. For a set of local interventions $\{\tau_{X_i}^{k_{X_i}}\}$, writing $\tau_S^{k_S}$ denotes the product of local interventions with k_S the tuple of outcomes. In general, if not specified to be local interventions, $\tau_S^{k_S}$ may be a global intervention with (single) outcome k_S. Finally, for a bipartition of nodes $S \subseteq \{X_1, \ldots, X_n\}$ and $R := \{X_1, \ldots, X_n\} \setminus S$, and a fixed intervention τ_R at the R nodes, the marginal process is denoted $\kappa_S^{\tau_R} = \sum_R (\kappa_{SR}\, \tau_R)$. It is understood that writing κ_S, where the intervention is suppressed in the superscript, indicates the 'no intervention' at the marginalised nodes, i.e. $\kappa_S = \sum_R (\kappa_{SR}\, \tau_R^{\text{id}})$.

5.3.2 Classical split-node causal models

Within the formalism of classical processes there is also then a natural notion of a causal model, which parallels that of a quantum causal model from Def. 5.1, and which is called a *classical split-node causal model*[5].

Definition 5.6 (Classical split-node causal model): *A* Classical split-node causal model *(CSM) is given by:*

(1) *a causal structure represented by a DAG G with vertices corresponding to classical split-nodes $X_1, ..., X_n$,*

(2) *for each X_i, a classical channel $P(X_i^{in}|Pa(X_i)^{out})$.*

The CSM defines a classical process map over the classical split nodes $X_1, \ldots, X_n$, given by

$$\kappa_{X_1 \cdots X_n} \;=\; \prod_i P(X_i^{in}|Pa(X_i)^{out}) \; . \tag{5.16}$$

Similarly to ordinary classical causal models and the quantum case, the definition expresses the idea that, if the causal structure between the classical split nodes $X_1, \ldots, X_n$ is as given by the DAG G with vertices $X_1, \ldots, X_n$, then such assertion constrains the classical process $\kappa_{X_1 \ldots X_n}$ that effectively describes the nodes $X_1, \ldots, X_n$. That constraint is the corresponding Markov condition for classical processes, which allows reference to a CSM as the pair $(G, \kappa_{X_1 \ldots X_n})$ of a DAG G with vertices $X_1, \ldots, X_n$ and a classical process $\kappa_{X_1 \ldots X_n}$ that is Markov for G.

Definition 5.7 (Classical split-node Markov condition): *A classical process $\kappa_{X_1 \ldots X_n}$ is called* Markov *for a DAG G with classical split nodes $X_1, \ldots, X_n$ as its vertices if and only if it admits a factorization into classical channels of the form $\kappa_{X_1 \ldots X_n} = \prod_i P(X_i^{in}|Pa(X_i)^{out})$.*

[5] They were first introduced in Ref. [4] as 'classical interventional models'.

An analogous analysis to that in Sec. 5.2 could be presented to justify the definition of classical split-node causal models. This would combine the notion of classical causal relations from Sec. 3.1.2 in terms of dependences between variables in an underlying functional model with the approach from Chap. 4 for lifting such notions to the level of nodes and processes, in this case classical processes. However, this is straightforward, little insightful and therefore omitted.

The next subsection will put the new definitions to their main purpose — elucidate the relation between quantum and classical causal models.

5.3.3 Overview: the trinity of causal models

The relationships between quantum, classical split-node and classical causal models, are described below. To ease frequent reference in later sections they are labelled as the set of relations $I_{\sigma\to\kappa}$, $I_{\kappa\to\sigma}$, $I_{\kappa\to P}$ and $I_{CCM\to CSM}$, which spell out how certain data *induces* other data. Crucially, the first three of them are primarily just relations between the three kinds of objects given by quantum processes over quantum *i*nodes, classical processes and probability distributions over classical variables and make sense independent of any causal assumptions.

$I_{\sigma\to\kappa}$ Given a process operator $\sigma_{A_1\ldots A_n}$, suppose that there exists an orthonormal basis at each node (that is, an orthonormal basis for $\mathcal{H}_{A_i^{\text{in}}}$ along with, noting Def. 3.11, the dual basis for $\mathcal{H}^*_{A_i^{\text{out}}}$), such that $\sigma_{A_1\ldots A_n}$ is diagonal with respect to the product of these bases. Then the process operator defines a classical process map, with in and out variables X_i^{in}, X_i^{out} at the ith node labelling the basis elements of $\mathcal{H}_{A_i^{\text{in}}}$ and $\mathcal{H}^*_{A_i^{\text{out}}}$, and the diagonal entries of $\sigma_{A_1\ldots A_n}$ interpreted as $P(X_1^{\text{in}},\ldots,X_n^{\text{in}}|X_1^{\text{out}},\ldots,X_n^{\text{out}})$. If the process operator is Markov for a particular DAG over $A_1,\ldots,A_n$, then the induced classical process map is Markov for the equivalent DAG over $X_1,\ldots,X_n$.

$I_{\kappa\to\sigma}$ A classical process map straightforwardly induces a quantum process operator by interpreting the variables X_i^{in} and X_i^{out} as labelling the elements of an orthonormal basis of $\mathcal{H}_{A_i^{\text{in}}}$, and its dual basis of $\mathcal{H}^*_{A_i^{\text{out}}}$, respectively, and by encoding the conditional probabilities $P(X_1^{\text{in}},\ldots,X_n^{\text{in}}|X_1^{\text{out}},\ldots,X_n^{\text{out}})$ as the diagonal elements of a matrix, which is then interpreted as a process operator $\sigma_{A_1\ldots A_n}$. If the classical process map is Markov for a particular DAG over $X_1,\ldots,X_n$, then the induced process operator is Markov for the equivalent DAG over $A_1,\ldots,A_n$.

$I_{\kappa \to P}$ A classical process map $\kappa_{X_1 \ldots X_n}$ straightforwardly induces a classical probability distribution $P(X_1, \ldots, X_n)$ by identifying input with output variables, marginalizing over the input variables to obtain

$$P(X_1^{\text{out}}, \ldots, X_n^{\text{out}}) = \sum_{X_1^{\text{in}} \ldots X_n^{\text{in}}} \left(\kappa_{X_1 \ldots X_n} \prod_i \delta(X_i^{\text{in}}, X_i^{\text{out}}) \right),$$

and then identifying each variable X_i^{out} with a single variable X_i such that $P(X_1, \ldots, X_n) = P(X_1^{\text{out}}, \ldots, X_n^{\text{out}})$. If the classical process map is Markov for a particular DAG over classical split nodes $X_1, \ldots, X_n$, then the probability distribution $P(X_1, \ldots, X_n)$ is Markov for the equivalent DAG over random variables $X_1, \ldots, X_n$.

$I_{CCM \to CSM}$ Given a classical causal model, with DAG G and channels $P(X_i|Pa(X_i))$, a classical split-node causal model is straightforwardly induced by replacing each variable X_i with the pair $X_i^{\text{in}}, X_i^{\text{out}}$, and by replacing the channels $P(X_i|Pa(X_i))$ with $P(X_i^{\text{in}}|Pa(X_i)^{\text{out}})$.

This makes precise *how*, as previously claimed, quantum causal models generalise classical causal models: the latter are formally special cases of the former via $I_{CCM \to CSM}$ and $I_{\kappa \to \sigma}$.

Note that while CSMs and CCMs are in 1-to-1 correspondence and thus define equivalent frameworks, they encode causal information in different ways. This is reflected in how $I_{CCM \to CSM}$ differs from the other three inductions — it only relates respective types of models. A probability distribution $P(X_1, \ldots, X_n)$ on its own does not allow for predictions for any intervention if not accompanied by the assertion of a causal DAG (for which it is Markov) and cannot induce a classical process $\kappa_{X_1 \ldots X_n}$, which does allow predictions for arbitrary interventions. However, the fact that not any classical process via $I_{\kappa \to P}$ yields a classical causal model, in turn succinctly expresses why classical processes, or quantum processes for that matter, in general fail to be causal models even though they are 'fully predictive' (see discussion in Sec. 3.2.4).

The following scheme summarises the relations, when applied to the respective types of causal models.

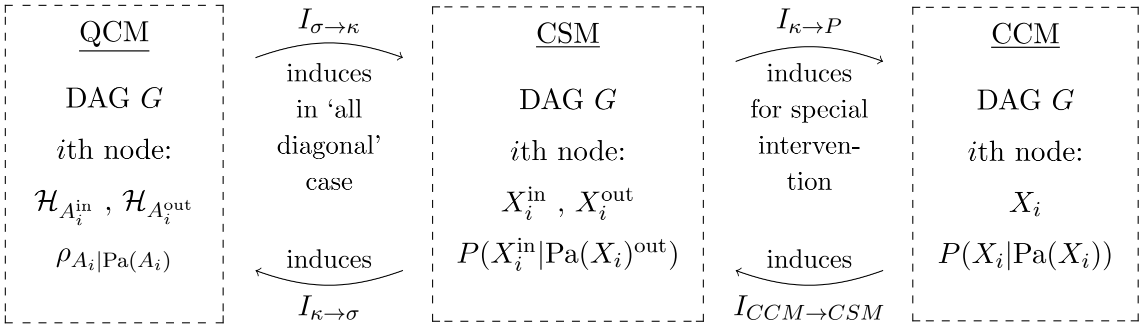


Figure 5.5: Summary of the relationships between QCMs, CSMs and CCMs.

5.3.4 Quantum and classical split-node do-interventions

In the context of classical causal models do-interventions play a crucial role (see Sec. 3.1). Typically it is also the only type of external intervention that is considered. In contrast, in the formalisms of quantum and classical processes all conceivable interventions are treated on the same footing and are equally important. Nonetheless, there are corresponding natural analogues to the classical do-intervention, which capture the idea of overriding the causal mechanism, which would otherwise fix the output state. A *quantum do-intervention* at node A ignores whatever state comes in at A^{in} and prepares some fixed state to be sent out at A^{out}, i.e. is of the form $\tau_A = \rho_{A^{\text{out}}} \otimes \mathbb{1}_{A^{\text{in}}}$ for some state $\rho_{A^{\text{out}}} \in \mathcal{L}(\mathcal{H}^*_{A^{\text{out}}})$. Similarly, in the classical split-node case. It will prove useful to introduce the following concept.

Definition 5.8 (do-conditional process operator): *Consider a set of quantum nodes V, with $S \subset V$ and $T = V \setminus S$, and let σ_{ST} be a process operator over the nodes in V. The* do-conditional process operator *for a do-intervention on S is given by*

$$\sigma_{Tdo(S)} \ := \ \text{Tr}_{S^{in}}[\sigma_{ST}]. \tag{5.17}$$

A do-conditional operator[6] $\sigma_{Tdo(S)}$ acts on $\mathcal{H}_{T^{\text{in}}} \otimes \mathcal{H}^*_{T^{\text{out}}} \otimes \mathcal{H}^*_{S^{\text{out}}}$ and can be thought of as representing 'half a do-intervention' at the S nodes, that is, it still awaits states to be fed in at the output spaces of the S nodes, to give back the marginal process operator on the T nodes.

Suppose the process $\sigma_{A_1\ldots A_n}$ is Markov for some DAG G, i.e. it holds that $\sigma_{A_1\ldots A_n} = \prod_i \rho_{A_i|Pa(A_i)}$. Then for any bi-partition of $\{A_1, \ldots, A_n\}$ into sets S and

[6]A similar idea appeared in Ref. [124] in the definition of what therein is called a 'quantum evolution map', however, not being in the context of quantum processes over quantum nodes, it does not allow to consider do-interventions at an arbitrary subset of nodes.

T, the do-conditional operator $\sigma_{Tdo(S)}$ simply becomes $\prod_{A_i \in T} \rho_{A_i|Pa(A_i)}$, reminiscent of the truncated factorisation formula in Eq. (3.3).

The analogue for a classical process κ_{ST} for disjoint sets of classical split nodes S and T is a *do-conditional classical process map* defined by

$$\kappa_{Tdo(S)} = \sum_{S^{\text{in}}} \kappa_{ST} \ .$$

Note that in the formulation of $I_{\kappa \to P}$ a choice was made to sum over the input spaces rather than the output spaces, which can now be seen to also ensure that the definition of $\kappa_{Tdo(S)}$ plays well with the 'limit' under $I_{\kappa \to P}$, namely that one recovers $P(T|do(S))$. Writing $\kappa_{Tdo(S=s)}$ has the obvious meaning, i.e. $\kappa_{Tdo(S=s)} = \sum_{S^{\text{out}}} \left[\kappa_{Tdo(S)} \ \delta(S^{\text{out}}, s) \right]$.

Given a quantum (classical) process, for any choice of a subset of nodes, the do-conditional operator (process map) is always defined, independent of whether the given data is part of a causal model or not. This fact emphasises again the key difference in encoding causal knowledge between CCMs, on the one hand, and CSMs and QCMs, on the other hand.

5.4 Notions of independence

This section presents notions of independence that generalise the classical notions of unconditional and conditional statistical independence to genuinely quantum ones. This is to say, they come as constraints at the quantum level of description — in terms of process operators — rather than probability distributions that arise from quantum systems.

Classically, causal structure imposes constraints in the form of conditional independence relations, and making this link precise is a core part of the framework of causal models (see Sec. 3.1.3). However, conditional independence is defined at the level of probability distributions and a core concept in statistics independent from causal models. Similarly, the following analysis is done independently from causal assumptions — 'quantum independence relations' may hold without being enforced through causal constraints and should be meaningful as such. The interplay with causal claims will be studied in Sec. 5.5. The analysis proceeds by reiterating known concepts for classical probability distributions and ordinary quantum states, to then generalise them via classical processes to quantum processes. Studying classical processes turns out to not only be a helpful pedagogical intermediate step, but also insightful in its own right.

5.4.1 2-place independence relations

5.4.1.1 Classical probability distributions

Given a probability distribution $P(Y, Z)$, recalling from Sec. 3.1.3, the (sets of) variables Y and Z are statistically independent, written $(Y \perp\!\!\!\perp Z)_P$, if and only if $P(Y, Z) = P(Y)P(Z)$.

5.4.1.2 Quantum states

Given a quantum state ρ_{AB}, the (sets of) systems A and B are independent, written $(A \perp\!\!\!\perp B)_{\rho_{AB}}$, if and only if $\rho_{AB} = \rho_A \otimes \rho_B$. This condition is equivalent to that for arbitrary local measurements at A and B with outcomes k_A and k_B, respectively, it holds that $P(k_A, k_B) = P(k_A)P(k_B)$. This is why the quantum systems A and B are sometimes also said to be uncorrelated in that case.

5.4.1.3 Classical processes

For classical processes, there are two inequivalent notions of independence. A first one is the following.

Definition 5.9 (Classical strong independence): *Given a classical process κ_{YZ}, the (sets of) classical split nodes Y and Z are* strongly independent*, written $(Y \perp\!\!\!\perp Z)_{\kappa_{YZ}}$, if and only if $\kappa_{YZ} = \kappa_Y \kappa_Z$.*

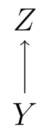
It has the operational meaning expected for the independence between nodes of a classical process.

Proposition 5.1 *Given a classical process κ_{YZ}, the condition $(Y \perp\!\!\!\perp Z)_{\kappa_{YZ}}$ holds if and only if for all local interventions at Y and Z, with outcomes k_Y and k_Z, respectively, the probability distribution $P(k_Y, k_Z)$ satisfies $(k_Y \perp\!\!\!\perp k_Z)_P$.*

Since Prop. 5.1 is a special case of Prop. 5.2, no separate proof is stated. Due to the equivalence in Prop. 5.1, strong independence can be understood as 'uncorrelated outcomes' for arbitrary interventions if agents were stationed at all nodes. The following weaker notion can then be seen as a notion of independence between the systems themselves that are associated with the nodes when not considering any interventions.

Definition 5.10 (Classical weak independence): *Given a classical process κ_{YZ}, let $P(Y, Z)$ be the probability distribution over the sets of single variables Y and Z, obtained via $I_{\kappa \to P}$. The sets of classical split nodes Y and Z are* weakly independent *if and only if $P(Y, Z) = P(Y)P(Z)$.*

Clearly, strong independence implies weak independence since the 'no intervention' of $I_{\kappa \to P}$ can be seen as a special kind of intervention. That the converse does not hold is established by the following example.



$$Z^{\text{in}} = Y^{\text{out}} \ ,$$

$$P(Y^{\text{in}} = 0) = 1 \ .$$

Figure 5.6: Example, where weak independence holds but strong independence does not.

Suppose a classical process κ_{YZ} over two classical split nodes Y and Z with binary input and output variables is given by the scenario in Fig. 5.6, that is, Z^{in} is fixed to be the same as Y^{out} and Y^{in} is fixed to be 0. This 'fine-tuned' point distribution $P(Y^{\text{in}})$ means that $P(Y, Z)$, obtained via $I_{\kappa \to P}$, also is a point distribution, which trivially takes a product form, establishing $P(Y, Z) = P(Y)P(Z)$. A generic intervention at Y, which prepares some probability distribution over Y^{out} will obviously lead to correlated outcomes at Y and Z due to $Z^{\text{in}} = Y^{\text{out}}$. Hence, strong independence, $(Y \perp\!\!\!\perp Z)_{\kappa_{YZ}}$, does not hold.

5.4.1.4 Quantum processes

A corresponding notion for quantum processes naturally is the following.

Definition 5.11 (Quantum strong independence): *Given a quantum process σ_{YZ}, the (sets of) quantum nodes Y and Z are* strongly independent*, written $(Y \perp\!\!\!\perp Z)_{\sigma_{YZ}}$, if and only if $\sigma_{YZ} = \sigma_Y \sigma_Z$.*

Recalling the restriction to quantum *i*nodes in this section, σ_Y and σ_Z are the marginal processes for 'no intervention' at the respective other nodes[7]. Also in the quantum case, strong independence has the expected operational meaning.

Proposition 5.2 *Given a quantum process σ_{YZ}, the condition $(Y \perp\!\!\!\perp Z)_{\sigma_{YZ}}$ holds if and only if for all local interventions at Y and Z, with outcomes k_Y and k_Z, respectively, the probability distribution $P(k_Y, k_Z)$ satisfies $(k_Y \perp\!\!\!\perp k_Z)_P$.*

[7] It is arguably the most natural way to define strong independence as $\sigma_{YZ} = \sigma_Y \sigma_Z$ for the marginal processes σ_Y and σ_Z, but $\sigma_{YZ} = \sigma_Y^{\tau_Z} \sigma_Z^{\tau_Y}$ is an equivalent statement no matter which choice of τ_Y, τ_Z.

Proof. See App. A.5. $\square$

By our convention of suppressing identity operators in products of the form $\sigma_Y \sigma_Z$, the latter is equal to $\sigma_Y \otimes \sigma_Z$, making $(A \perp\!\!\!\perp B)_{\rho_{AB}}$ for ordinary quantum states a special case. Furthermore, $(Y \perp\!\!\!\perp Z)_{\sigma_{YZ}}$ reduces to $(Y \perp\!\!\!\perp Z)_{\kappa_{YZ}}$ under $I_{\sigma \to \kappa}$. Whether a quantum analogue to classical weak independence exists, is left open.

5.4.2 3-place independence relations

5.4.2.1 Classical probability distributions

Given a probability distribution $P(Y, Z, W)$, recalling from Sec. 3.1.3, the (sets of) variables Y and Z are statistically independent conditional on W, written $(Y \perp\!\!\!\perp Z|W)_P$, if and only if $P(Y, Z|W = w) = P(Y|W = w)P(Z|W = w)$ whenever $P(W = w) \neq 0$. The following proposition, the proof of which is straightforward and omitted, reveals much of the guiding intuition for the below generalisations.

Proposition 5.3 *Given (sets of) variables Y, Z, W and a probability distribution $P(Y, Z, W)$, the following are equivalent:*

(1) $(Y \perp\!\!\!\perp Z|W)_P$.

(2) $P(Y, Z, W)\ P(W) = P(Y, W)\ P(Z, W)$.

(3) *There exist real functions $\alpha : Y \times W \to \mathbb{R}$ and $\beta : Z \times W \to \mathbb{R}$, such that $P(Y, Z, W) = \alpha(Y, W)\ \beta(Z, W)$.*

(4) *The conditional mutual information satisfies $I(Y : Z|W) = 0$.*

5.4.2.2 Quantum states

Given a quantum state ρ_{ABC} of three (sets of) systems A, B and C, define A and B to be *independent relative to C*, written $(A \perp\!\!\!\perp B|C)_{\rho_{ABC}}$, if and only if the quantum conditional mutual information between A and B given C vanishes, $I(A : B|C) = 0$. Note that this terminology refrains from speaking of 'quantum conditional independence', because 'conditioning on' invokes classical associations of variables, whose values can be considered fixed.

Before formulating a generalisation at the level of quantum processes, it will be instructive to introduce the following product of operators (see, e.g., Refs. [76, 125, 126]):

$$\star \quad : \quad \mathcal{L}(\mathcal{H}) \times \mathcal{L}(\mathcal{H}) \to \mathcal{L}(\mathcal{H})$$

$$(A, B) \;\mapsto\; A \star B := \lim_{n\to\infty} \left(A^{1/n}\, B^{1/n}\right)^n \; . \tag{5.18}$$

Among its useful properties are that it is associative and commutative, and reduces to the ordinary product AB if $[A, B] = 0$. For the special case of strictly positive definite operators, it holds that

$$A \star B = \exp(\log(A) + \log(B)) \; , \tag{5.19}$$

which can be generalised to positive semi-definite operators A and B in form of $\log(A \star B) = \log(A) + \log(B)$, where the logarithms are understood to be restricted to the supports of the respective operators [126]. We extend our convention of suppressing identity operators and write $\sigma_{XY} \star \sigma_{YZ}$ as short-hand for $(\sigma_{XY} \otimes \mathbb{1}_Z) \star (\mathbb{1}_X \otimes \sigma_{YZ})$.

An analogue to Prop. 5.3 for quantum states can now be stated as follows.

Proposition 5.4 *Given (sets of) systems A, B, C, and a quantum state ρ_{ABC}, the following are equivalent:*

(1) $(A \perp\!\!\!\perp B|C)_{\rho_{ABC}}$.

(2) $\rho_{ABC} \star \rho_C = \rho_{AC} \star \rho_{BC}$.

(3) *There exist Hermitian operators α_{AC} and β_{BC}, such that $\rho_{ABC} = \alpha_{AC}\, \beta_{BC}$.*

(4) *The Hilbert space $\mathcal{H}_C$ decomposes as $\mathcal{H}_C = \bigoplus_i \mathcal{H}_{C_i^L} \otimes \mathcal{H}_{C_i^R}$, such that $\rho_{ABC} = \sum_i q_i \left(\rho_{AC_i^L} \otimes \rho_{BC_i^R}\right)$, where $0 \leq q_i \leq 1$, $\sum_i q_i = 1$, and for each i, $\rho_{AC_i^L}$ and $\rho_{BC_i^R}$ are density operators on the Hilbert spaces indicated by the subscripts.*

If (3) *holds, then* $[\alpha_{AC}, \beta_{BC}] = 0$.

Proof. For '(1) $\Leftrightarrow$ (2)', see Refs. [76, 127]. For '(1) $\Leftrightarrow$ (4)', see Ref. [122]. It is immediate that '(4) $\Rightarrow$ (3)' and straightforward to verify that '(3) $\Rightarrow$ (2)'. If $\rho_{ABC} = \alpha_{AC}\, \beta_{BC}$, for Hermitian α_{AC} and β_{BC}, then taking the Hermitian conjugate of both sides of the equation yields $[\alpha_{AC}, \beta_{BC}] = 0$. □

5.4.2.3 Classical processes

Inspired by Prop. 5.3, classical strong independence naturally lifts to a 3-place relation.

Definition 5.12 (Classical strong relative independence): *Given a classical process κ_{YZW}, say that Y* and *Z* are strongly independent relative to *W, written*

$(Y \perp\!\!\!\perp Z \mid W)_{\kappa_{YZW}}$, *if and only if there exist real functions* $\alpha_{YW} : Y^{in} \times Y^{out} \times W^{in} \times W^{out} \to \mathbb{R}$ *and* $\beta_{ZW} : Z^{in} \times Z^{out} \times W^{in} \times W^{out} \to \mathbb{R}$*, such that* $\kappa_{YZW} = \alpha_{YW}\ \beta_{ZW}$*.*

Clearly, $(Y \perp\!\!\!\perp Z|W)_{\kappa_{YZW}}$ reduces to $(Y \perp\!\!\!\perp Z)_{\kappa_{YZ}}$ for $W = \emptyset$. The reason for the terminology of strong independence 'relative to' W, despite the presence of classical variables, which one could conceivably condition on, in contrast to the quantum case from Sec. 5.4.2.2, is that it does not make sense to 'condition on' W as a classical *split node*, or a set of such.

In order to give strong relative independence an operational reading, the following concept is needed.

Definition 5.13 (Maximally informative intervention): *A* maximally informative intervention *at a node* W*, with outcome* k_W*, is a classical intervention such that* W^{in} *and* W^{out} *can each be inferred from* k_W*. A necessary and sufficient condition is that:*

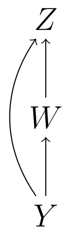
$$P(k_W, W^{out}|W^{in}) = \delta\big(g^{in}(k_W), W^{in}\big)\ \delta\big(g^{out}(k_W), W^{out}\big)\ P(k_W, W^{out}|W^{in})\ ,$$

where g^{in} *is a surjective function and* g^{out} *an arbitrary function. For* W *a set of nodes, a maximally informative local intervention at* W *is a product of maximally informative interventions at each node in* W*.*

Proposition 5.5 *Given a classical process* κ_{YZW}*, the condition* $(Y \perp\!\!\!\perp Z|W)_{\kappa_{YZW}}$ *holds if and only if for any choice of maximally informative local intervention at* W *with outcome* k_W*, and any local interventions at* Y *and* Z*, with outcomes* k_Y *and* k_Z*, respectively, the joint probability distribution* $P(k_Y, k_Z, k_W)$ *satisfies* $(k_Y \perp\!\!\!\perp k_Z|k_W)_P$*.*

Proof. See Appendix A.6. □

If an agent performs a maximally informative local intervention at the W nodes, then, upon obtaining some outcome k_W, she knows with certainty the values of all $W^{\rm in}$ and $W^{\rm out}$, which are supposedly the only variables, which 'underwrite correlation between Y and Z' — so at least the intuition of conditional independence type relations. Hence, that $(Y \perp\!\!\!\perp Z|W)_{\kappa_{YZW}}$ implies the above operational statement is as expected. Note that the operational statement could not be weakened by restriction to 'perfect, non-disturbing' measurements of the form $\delta(k_W, W^{\rm in})\delta(W^{\rm out}, W^{\rm in})$. Interventions that relate distinct values of $W^{\rm out}$ and $W^{\rm in}$ are essential for establishing equivalence. See Fig. 5.7 for an example.



$$Z^{\text{in}} = Y^{\text{out}} \oplus W^{\text{out}} \ ,$$

$$W^{\text{in}} = Y^{\text{out}} \ ,$$

$$P(Y^{\text{in}}) \ .$$

Figure 5.7: Example of a classical process over 3 split nodes with all variables being bits, valued in $\{0,1\}$, and defined by the shown functions, where $\oplus$ is addition modulo 2. ($P(Y^{\text{in}})$ left unspecified as irrelevant.) For the 'perfect, non-disturbing' measurement $\delta(k_W, W^{\text{in}})\delta(W^{\text{out}}, W^{\text{in}})$ it ends up being the case that $Z^{\text{in}} = 0$ is fixed and, hence, $(k_Y \perp\!\!\!\perp k_Z | k_W)_P$ holds for arbitrary interventions at Y and Z. However, $(k_Y \perp\!\!\!\perp k_Z | k_W)_P$ clearly fails for some maximally informative intervention at W.

Also weak independence from Def. 5.10 lifts to a 3-place relation and inherits its logical relationship to strong relative independence from the special cases for $W = \emptyset$.

Definition 5.14 (Classical weak relative independence): *Given a classical process* κ_{YZW}*, let* $P(Y,Z,W)$ *be the joint probability distribution over sets of single variables* Y,Z,W *obtained via* $I_{\kappa \to P}$*. For the sets of classical split nodes,* Y and Z are weakly independent relative to W *if and only if* $(Y \perp\!\!\!\perp Z|W)_P$*.*

Importantly, strong and weak relative independence are both conditions on a classical process. While $(Y \perp\!\!\!\perp Z|W)_{\kappa_{YZW}}$ reduces to $(Y \perp\!\!\!\perp Z|W)_P$ under $I_{\kappa \to P}$ (noting Prop. 5.3), the fact that the converse does not hold is independent from the logical relation between strong and weak relative independence. If $(Y \perp\!\!\!\perp Z|W)_P$ holds for a given probability distribution $P(Y,Z,W)$, there is no induced classical process for which either strong or weak relative independence could obtain.

5.4.2.4 Quantum processes

Finally, one arrives at the following quantum analogue of classical conditional independence that, inspired by Prop. 5.4, lifts quantum strong independence to a 3-place relation.

Definition 5.15 (Quantum strong relative independence): *Given a quantum process* σ_{YZW}*, say that* Y is strongly independent from Z relative to W*, and written* $(Y \perp\!\!\!\perp Z|W)_{\sigma_{YZW}}$*, if and only if there exist Hermitian operators* α_{YW} *and* β_{ZW} *such that*

$$\sigma_{YZW} \ = \ \alpha_{YW} \, \beta_{ZW} . \tag{5.20}$$

Here, just as with process operators, the label of a (set of) quantum nodes A in the subscript of a Hermitian operator α_A indicates that $\alpha_A \in \mathcal{L}(\mathcal{H}_{A^{\text{in}}} \otimes \mathcal{H}^*_{A^{\text{out}}})$. Strong independence $(Y \perp\!\!\!\perp Z)_{\sigma_{YZ}}$ is subsumed as the special case $W = \emptyset$. Classical strong relative independence, $(Y \perp\!\!\!\perp Z|W)_{\kappa_{YZW}}$, is recovered under $I_{\sigma\to\kappa}$ [8], and conversely, becomes a special case of the quantum version via $I_{\kappa\to\sigma}$.

Concerning the operational meaning of $(Y \perp\!\!\!\perp Z|W)_{\sigma_{YZW}}$, the situation is more subtle than with the classical analogue. The reason is that there is no quantum analogue of a maximally informative intervention (Def. 5.13), which could be performed at the W nodes so as to reveal the 'value they have'. The following presents an operational statement that is implied by, but not equivalent to $(Y \perp\!\!\!\perp Z|W)_{\sigma_{YZW}}$.

Proposition 5.6 *Consider a quantum process σ_{YZW}. If $(Y \perp\!\!\!\perp Z|W)_{\sigma_{YZW}}$, then there exists a global intervention at the W nodes, with outcome k_W, such that for all local interventions at Y, Z, with joint outcomes k_Y, k_Z, respectively, the joint probability distribution $P(k_Y, k_Z, k_W)$ satisfies $(k_Y \perp\!\!\!\perp k_Z|k_W)_P$.*

Proof. Suppose that $\sigma_{YZW} = \alpha_{YW}\,\beta_{ZW}$. Due to Lem. 4.1, the commutation of α_{YW} and β_{ZW} implies the existence of a decomposition $\mathcal{H}_{W^{\text{in}}} \otimes \mathcal{H}^*_{W^{\text{out}}} = \bigoplus_i \mathcal{H}_{F_i^L} \otimes \mathcal{H}_{F_i^R}$ into orthogonal subspaces such that $\sigma_{YZW} = \sum_i \alpha_{YF_i^L} \otimes \beta_{ZF_i^R}$ (note that α_{YW} and β_{ZW} can be chosen to be positive[9]). Let $\{|i, f_i^L\rangle\, |i, f_i^R\rangle\}_{f_i^L, f_i^R}$ be a product orthonormal basis of the ith subspace $F_i^L \otimes F_i^R$.

Consider the following global intervention at W. An agent is stationed at an additional locus E, such that for each node $N \in W$, the quantum system at N^{in} is sent to E, one of a maximally entangled pair of systems is fed into N^{out}, and the other one is sent to E. This defines a new quantum process σ_{YZE} over Y, Z and E, with E^{in} isomorphic to $\mathcal{H}_{W^{\text{in}}} \otimes \mathcal{H}_{W^{\text{out}}}$ (and hence to $\mathcal{H}_{W^{\text{in}}} \otimes \mathcal{H}^*_{W^{\text{out}}}$), such that σ_{YZE} has a block-diagonal structure with respect to the induced decomposition. Let $|i, f_i^L, f_i^R\rangle := J^{-1}\, |i, f_i^L\rangle\, |i, f_i^R\rangle$ label the induced orthonormal basis of E^{in} (for a suitable isomorphism J). The agent performs the von Neumann measurement at E corresponding to that basis. For a particular outcome k_E, corresponding to the

[8]One might worry that, in case of degenerate eigenbases, it is not obvious that α_{YW} and β_{ZW} can be chosen to be diagonal in the same fixed basis in which σ_{YZW} defines the classical process. See, e.g., Prop. 5.7 together with Rem. 5.2 for that $(Y \perp\!\!\!\perp Z|W)_{\kappa_{YZW}}$ is indeed recovered under $I_{\sigma\to\kappa}$ given that quantum strong relative independence holds for κ_{YZW} (seen as a quantum process).

[9]Strictly speaking, Lem. 4.1 is formulated for commuting operators which are correctly normalised as CJ representations of channels, while here α_{YW} and β_{ZW} are only assumed to be positive. It is, however, easy to see that nothing in the proof of that lemma changes if one accounts for different normalisation everywhere.

basis state $|i, f_i^L, f_i^R\rangle$, define the operator

$$\begin{aligned}\mathrm{Tr}_E\Big[\sigma_{YZE}\ |i, f_i^L, f_i^R\rangle\langle i, f_i^L, f_i^R|\Big] \\ &= d_{E^{\mathrm{out}}}\ \langle i, f_i^L, f_i^R|\ J^{-1}\Big(\sum_j \alpha_{YF_j^L}\otimes\beta_{ZF_j^R}\Big)J\ |i, f_i^L, f_i^R\rangle \\ &= d_{E^{\mathrm{out}}}\ \langle i, f_i^L|\,\alpha_{YF_i^L}\,|i, f_i^L\rangle\ \otimes\ \langle i, f_i^R|\,\beta_{ZF_i^R}\,|i, f_i^R\rangle\ =:\ \gamma_Y\otimes\eta_Z\ ,\end{aligned}$$

where the $d_{E^{\mathrm{out}}}$ results from the trace over E^{out}, on which σ_{YZE} acts trivially, and is then absorbed into, say γ_Y. The product form $\gamma_Y\otimes\eta_Z$ implies that the joint probability distribution for k_E and outcomes k_Y and k_Z for arbitrary choices of interventions at Y and Z satisfies $P(k_Y, k_Z, k_E) = \phi(k_Y, k_E)\chi(k_Z, k_E)$ (for some functions ϕ and χ). Recalling Prop. 5.3, this establishes the claim. □

In order to see that the converse does indeed not hold, consider the following simple example with three quantum systems A, B and C, all two-dimensional, and let $\rho_{BC|A}$ be the channel corresponding to the coherent copy map that takes $|i\rangle$ to $|i\rangle|i\rangle$ for the computational basis $i = 0, 1$ (also see Sec. 3.2.5.1 for this example). Seeing A, B and C as quantum nodes, then it is true that there exists an intervention at A, namely the von Neumann measurement in the computational basis, such that conditional on its outcome i, the outcomes k_B and k_C will be independent for arbitrary measurements at B and C. However, for arbitrary states ρ_A one finds that for the quantum process $\sigma_{ABC} = \rho_{BC|A}\ \rho_A$, the relation $(B \perp\!\!\!\perp C|A)_{\sigma_{ABC}}$ fails [4].

Whether there is an insightful operational statement that is equivalent to strong relative independence, as well as, whether there is a weak notion of quantum relative independence are left open.

Observe that also in the case of quantum processes there are equivalent statements, analogous to those in Propositions 5.3 and 5.4. Since needed here and frequently in the subsequent sections, given a process operator $\sigma_{A_1\ldots A_n}$, let $\hat{\sigma}_{A_1\ldots A_n}$ denote the corresponding operator that is correctly normalised as a trace-1 quantum state on the $2n$ Hilbert spaces, i.e. $\hat{\sigma}_{A_1\ldots A_n} = \frac{1}{\prod_i d_{A_i^{\mathrm{out}}}}\sigma_{A_1\ldots A_n}$.

Proposition 5.7 *Let σ_{YZW} be a process operator. The following are equivalent:*

(1) $(Y \perp\!\!\!\perp Z|W)_{\sigma_{YZW}}$.

(2) $\sigma_{YZW}\ \star\ \sigma_W^{\tau_Y\tau_Z}\ =\ \sigma_{YW}^{\tau_Z}\ \star\ \sigma_{ZW}^{\tau_Y}\qquad\forall$ local interventions $\tau_Y,\ \tau_Z$.

(3) $I(Y : Z|W) = 0$, *evaluated on $\hat{\sigma}_{YZW}$, the trace-1 operator obtained from σ_{YZW} as defined above.*

Proof. This proposition is a special case of Prop. 5.10 (see proof in App. A.9). □

Remark 5.2 *Note that a set of completely analogous equivalent statements hold for classical strong relative independence,* $(Y \perp\!\!\!\perp Z|W)_{\kappa_{YZW}}$*, just replacing* σ_{YZW} *with* κ_{YZW} *everywhere, replacing the '*$\star$*'-product in (2) with ordinary multiplication of functions and* $I(Y : Z|W)$ *in (3) with the classical conditional mutual information. The proof is analogous.*

5.5 A quantum d-separation theorem

The previous section presented novel notions of independence, in particular a quantum analogue of conditional statistical independence. The immediate question, the present section addresses, is how do these independence relations relate to causal claims.

As far as the classical case of probability distributions over variables is concerned, the d-separation theorem, presented in Sec. 3.1.3, exhaustively captures this link. If the set of vertices Y is d-separated from the set Z by the set W in a DAG G, denoted $(Y \perp\!\!\!\perp Z|W)_G$, then whenever a probability distribution P is Markov for G, then it holds $(Y \perp\!\!\!\perp Z|W)_P$. This is soundness of d-separation for conditional independence. Although the graphical property of d-separation (Def. 3.5) is somewhat involved, Sec. 3.1.3 showed how looking at the basic scenarios of fork, chain and collider makes it intuitive to expect $(Y \perp\!\!\!\perp Z|W)_P$ to hold, whenever the causal structure satisfies $(Y \perp\!\!\!\perp Z|W)_G$. That d-separation also is the best structural criterion possible to capture conditional independence relations, is established through the completeness part of the d-separation theorem.

When it comes to quantum systems, it was previously unclear and at times contested whether d-separation still provides the appropriate structural criterion of a causal kind that could capture 'quantum independence relations' (see Refs. [34, 80] and the discussion in Sec. 3.2.2). This essentially boils down to the same analysis which concludes a failure of Reichenbach's common cause principle due to Bell's theorem, i.e. the fact that we do observe correlation between parties A and B conditioned on the successful preparation of a Bell-state at P, although the fork $A \leftarrow P \rightarrow B$ is a canonical example of A and B being d-separated by P. The main idea behind the quantum common cause principle (Principle 2) from Ref. [4] and the general programme pursued in this thesis is that there is nothing wrong with the above causal assertion of $A \leftarrow P \rightarrow B$, nor with that it ought to impose quantitative constraints, but with the terms in which the constraints are formulated. Conditional independence relations in probability distributions, which arise from quantum systems through interventions, is not the right level to look for the ramifications of d-separation properties in the underlying causal structure. In contrast, quantum strong relative independence from Def. 5.15 is a genuinely quantum notion and might satisfy a d-separation theorem. That this is indeed the case is established in the following.

A standard tool in this context uses the *semi-graphoid axioms*, which axiomatise the logical relationship between conditional independence type statements [97, 128]. Given a set V and a 3-place relation S on the subsets of V, letting $Y, Z, W, X \subseteq V$ be arbitrary disjoint subsets, the semi-graphoid axioms are:

$$\begin{aligned} &\text{symmetry} && S(Y,Z;W) \;\Leftrightarrow\; S(Z,Y;W)\;, && (5.21)\\ &\text{decomposition} && S(Y,XZ;W) \;\Rightarrow\; S(Y,Z;W)\;, && (5.22)\\ &\text{weak union} && S(Y,XZ;W) \;\Rightarrow\; S(Y,Z;XW)\;, && (5.23)\\ &\text{contraction} && S(Y,Z;W)\,\wedge\, S(Y,X;ZW) \;\Rightarrow\; S(Y,ZX;W)\;. && (5.24) \end{aligned}$$

A *semi-graphoid* is a model given by a set V and a relation S that satisfies these four axioms. Furthermore, a 3-place relation S on the subsets of V satisfies the *local Markov condition* relative to a DAG G with vertices V if and only if

$$\forall X \in V\;, \qquad S(\{X\}, Nd(X)\setminus Pa(X); Pa(X))\;, \tag{5.25}$$

where $Nd(X)$ denotes the non-descendants of X. The intuition behind this property, interpreting the 3-place relation S as a conditional independence type relation, is that the parents of X screen X off its non-descendants. For a semi-graphoid S on V, the local Markov condition relative to the DAG G is equivalent to what is called the 'global Markov condition' for G [96, 129], namely,

$$(Y \perp\!\!\!\perp Z|W)_G \;\Rightarrow\; S(Y,Z;W)\;. \tag{5.26}$$

It is now crucial to note that these general results from the literature, just as the specific d-separation theorem for classical conditional independence (Thm. 3.2), concern a 3-place relation that is defined on arbitrary triples of disjoint subsets of a set V. Given a quantum process $\sigma_{A_1\ldots A_n}$ on a set of quantum nodes $A_1,\ldots,A_n$, there however is an ambiguity for how to calculate a marginal process over a triple of disjoint subsets Y, Z, W. Let $R := \{A_1,\ldots,A_n\}\setminus(Y\cup Z\cup W)$. Whether $\sigma^{\tau_R}_{YZW}$ satisfies $(Y \perp\!\!\!\perp Z|W)_{\sigma^{\tau_R}_{YZW}}$ or not, will in general depend on the intervention τ_R at the R nodes. This is just as it does classically, but given a probability distribution, there is no such ambiguity over marginalisation, because a probability distribution just does not allow to answer the question for interventions on the remaining variables.

In order to define an unambiguous relation that can be evaluated for arbitrary triples of disjoint subsets Y, Z, W, the following theorem will make the strongest possible choice: for the soundness part a quantification over all possible interventions at the R nodes, while the statement of the completeness part refers to the 'no intervention' at the remaining nodes, $\sigma_{YZW} = \sigma_{YZW}^{\tau_R^{\mathrm{id}}}$.

Theorem 5.3 (Quantum d-separation theorem): *Consider a DAG G, with a set V of quantum nodes, and disjoint subsets of nodes Y, Z, and W, with $R := V \setminus (Y \cup Z \cup W)$.*

(1) *(Soundness): If $(Y \perp\!\!\!\perp Z|W)_G$, then for any process operator σ_{YZWR} that is Markov for G, it holds that: for any local intervention τ_R at R, the marginal $\sigma_{YZW}^{\tau_R}$ satisfies $(Y \perp\!\!\!\perp Z|W)_{\sigma_{YZW}^{\tau_R}}$.*

(2) *(Completeness): If $(Y \not\perp\!\!\!\perp Z|W)_G$, then there exists a process operator σ_{YZWR} that is Markov for G, such that with no interventions at the R nodes, for the marginal σ_{YZW} it holds that $(Y \not\perp\!\!\!\perp Z|W)_{\sigma_{YZW}}$.*

Proof. Given a set of quantum nodes V, and a process operator σ_V, define the 3-place relation T on the subsets of V as

$$T(Y, Z; W) \qquad \text{iff} \qquad \forall \text{ local interventions } \tau_R, (Y \perp\!\!\!\perp Z|W)_{\sigma_{YZW}^{\tau_R}}. \qquad (5.27)$$

The soundness part of Thm. 5.3 follows from the following two lemmas.

Lemma 5.2 *Given a process operator σ_{YZWR}, the relation T defined by Eq. (5.27) satisfies the semi-graphoid axioms.*

Proof of Lem. 5.2. See App. A.7 □

Lemma 5.3 *Consider a DAG G, with nodes V, and a process operator σ_V that is Markov for G. The relation T defined by Eq. (5.27) satisfies the local Markov condition.*

Proof of Lem. 5.3. See App. A.7 □

Finally, for the completeness part of Thm. 5.3, consider a DAG G with quantum nodes V, and suppose that $(Y \not\perp\!\!\!\perp Z|W)_G$ for disjoint subsets of nodes Y, Z, and W. Let $R = V \backslash (Y \cup Z \cup W)$. Associate a classical random variable with each node, ranging over a set of values, whose cardinality is the same as the dimension of the input Hilbert space of the respective quantum node (equivalently, the dimension of the output Hilbert space, as quantum nodes are assumed to be *i*nodes). By virtue of the completeness part of Thm. 3.2, there exists a joint probability distribution $P(Y, Z, W, R)$ over these random variables, Markov for G, for which $(Y \not\perp\!\!\!\perp Z|W)_P$. This classical causal model induces a classical split-node causal model with the same DAG via $I_{CCM \to CSM}$ of Sec. 5.3, for which $(Y \not\perp\!\!\!\perp Z|W)_{\kappa_{YZW}}$. This in turn induces a quantum causal model with the same DAG via $I_{\kappa \to \sigma}$, for which $(Y \not\perp\!\!\!\perp Z|W)_{\sigma_{YZW}}$. This concludes the proof of Thm. 5.3. □

Seeing as we are here only considering quantum $\imath$nodes, there is another natural choice to arrive at an unambiguous 3-place relation defined on all triples of disjoint subsets of nodes, namely $(Y \perp\!\!\!\perp Z|W)_{\sigma_{YZW}}$, that is, instead of quantifying over all interventions at the remaining nodes, to always consider the 'no intervention'. By virtue of being a special case of the logically stronger statement in the above theorem, d-separation is sound for this relation. However, it is not entirely obvious and left open whether $(Y \perp\!\!\!\perp Z|W)_{\sigma_{YZW}}$ itself satisfies the contraction axiom, if marginals are calculated with the 'no intervention' throughout (the other three semi-graphoid axioms are straightforward).

Since classical strong and weak relative independence formally become special cases of quantum strong relative independence via $I_{\kappa \to \sigma}$, observe that Thm. 5.3 also gives that d-separation is sound and complete for classical strong and weak relative independence. This is again in the strongest possible sense, with quantifying over all possible interventions at the remaining nodes for the soundness part, and the completeness part only involving the 'no intervention' at the remaining nodes.

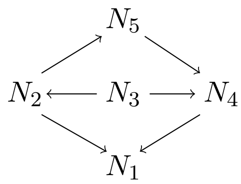


Figure 5.8: Example of a DAG G for illustration of Thm. 5.3.

In order to illustrate Thm. 5.3, consider the DAG G in Fig. 5.8. Suppose the quantum process $\sigma_{N_1 \dots N_5}$ is Markov for G. For instance, it holds that $(N_2 \perp\!\!\!\perp N_4|\{N_3, N_5\})_G$ and therefore $(N_2 \perp\!\!\!\perp N_4|\{N_3, N_5\})_{\sigma^{\tau_{N_1}}_{N_2 \dots N_5}}$ for all interventions τ_{N_1}. Note that since N_1 is a leaf node it does not matter at all which intervention for marginalisation is considered at N_1. With Prop. 5.6 it follows that there exists a (in this case even local) intervention at N_3 and N_5 such that conditioned on its outcome, the outcomes of arbitrary interventions at N_2 and N_4 are independent from each other. In contrast, consider for instance the fact that $(N_2 \not\perp\!\!\!\perp N_4|N_5)_G$. Indeed, once marginalised over the common cause N_3, as one would expect, in general there does not exist an intervention at N_5 that would lead to uncorrelated outcomes at Y and Z for arbitrary interventions.

We close with two remarks on differences between the classical and quantum case. First, it was mentioned above that for any semi-graphoid the local and global Markov condition relative to some DAG G are equivalent. For a classical probability distribution $P(X_1,\ldots,X_n)$ and conditional independence defining the semi-graphoid, these conditions are furthermore equivalent to the condition that $P(X_1,\ldots,X_n)$ factorises relative to G, as in what is just called the Markov condition according to Def. 3.2 (see, e.g., Ref. [9]). Note that an analogous equivalence does not hold in the quantum case. If $\sigma_{A_1\ldots A_n}$ is Markov for some DAG G, that is, 'factorises relative' to G according to Def. 5.2, then the local Markov condition from Eq. (5.25) and the global Markov condition from Eq. (5.26) hold with the 3-place relation given by T from Eq. (5.27). However, the converse is not true. Consider for instance a process σ_{ABC} on three quantum nodes of the form $\sigma_{ABC} = \rho_{C|A}\ \rho_{A|B}\ \rho_B$. This process is Markov for the chain $B \to A \to C$. Now, consider the DAG given by the fork $B \leftarrow A \to C$ and observe that the only constraint imposed by the global Markov condition for the fork is $(B \perp\!\!\!\perp C|A)_{\sigma_{ABC}}$. That the given process σ_{ABC} satisfies the latter condition is evident, while σ_{ABC} is not Markov for the fork.

Second, as mentioned in Chap. 3.1, the classical d-separation theorem can be understood independently from concerns about causal reasoning in the context of Bayesian networks. In particular, any distribution $P(X_1,\ldots,X_n)$ is Markov for many different DAGs, most of which cannot have anything to do with causal structure. Unsurprisingly, the situation is very different for quantum or classical processes due to their process nature. Here, the d-seperation theorem plays no role in classifying which DAGs a process is Markov for (see Sec. 5.7.2), while it still achieves an analogous formalisation of the link between causal claims and quantum relative independence relations.

5.6 Constraints from causal structure

A key strength of the framework of classical causal models that was highlighted in Sec. 3.1.4, is that Pearl's do-calculus [9] solves the problem of the identifiability of causal effects. This do-calculus tells us when and how to calculate $P(Y|do(X))$ — without actually performing the do-intervention — just from causal assumptions and observational data, even when there are unobserved causally relevant variables. A main theme in comparing classical and quantum causal models in this thesis has been the different ways, in which causal knowledge is encoded in the respective types of causal models. In contrast to a given distribution $P(X_1, \ldots, X_n)$, given a quantum process $\sigma_{A_1 \ldots A_n}$, or for that matter, a classical *process*, one can always calculate the marginal process on a subset $T \subseteq \{A_1, \ldots, A_n\}$ for a do-intervention at the complementary subset S. In particular, the do-conditional operator $\sigma_{T|do(S)}$, the analogue of $P(Y|do(X))$, can always be calculated (see Sec. 5.3.4). Hence, if the given data is a quantum process $\sigma_{A_1 \ldots A_n}$, the 'identifiability of causal effects' (see Sec. 3.1.4) is not an interesting problem.

The core of the do-calculus are the three rules in Theorem 3.3. Independent from being the rules of a calculus that is useful for identifying causal effects, they are results, which take the form that a particular d-separation property in a mutilated version of a given DAG G implies a statement that relates Bayesian conditional and do-conditional probability distributions, provided the distribution on all variables of G is Markov for G. Thus, the rules expose consequences from particular properties of causal structure. As such, the rules may of course have insightful analogues in the quantum framework.

The following presents such generalisations of all three rules to classical split-node and quantum causal models. They are generalisations in the following sense. First, for classical and quantum processes, the generalised rule takes the same logical form, that is, given a DAG G, the same graphical antecedent as in the corresponding rule in Thm. 3.3 implies a constraint on a process that is Markov for G. Second, these constraints on quantum and classical processes are such that the respective classical consequents from Thm. 3.3 are recovered under the inductions $I_{\sigma \to \kappa}$ and $I_{\kappa \to P}$. Furthermore, intuitive operational statements are presented, which are implied by the respective constraints in the case of quantum processes and equivalent to the respective constraints in the case of classical processes. So, given that a process is Markov for a DAG G — and only then it is consistent to assume G to be the causal structure of the nodes without ignoring relevant common causes — the generalised rules identify consequences of an empirical nature that necessarily hold for particular causal arrangements in G, but not for all processes that are Markov for *some* DAG. They are therefore an integral part of carving out what the framework of quantum causal models is. Beyond that, there might of course be a type of problem, other than the identifiability of causal effects, for which the generalisations are 'useful', however, the investigation of such a problem is left for future work.

5.6.1 Generalisation do-calculus rule 1

5.6.1.1 Classical probability distributions

For convenience, Rule 1 is restated here: if the probability distribution $P(...)$ is Markov for the DAG G, then for disjoint sets of nodes Y, Z, X, W it holds that

$$(Y \perp\!\!\!\perp Z|X, W)_{G_{\overline{X}}} \quad \Rightarrow \quad P(Y|do(X), Z, W) \;=\; P(Y|do(X), W) \;, \qquad (5.28)$$

where, recalling Sec. 3.1.4, $G_{\overline{X}}$ denotes the DAG obtained from G by removing all arrows incident on vertices in X. Note that Rule 1 is a generalisation of soundness of d-separation for conditional independence (see Thm. 5.3), since the consequent in Eq. (5.28) says that Y is independent from Z conditional on W in the post do-intervention probability distribution $P(\ldots|do(X))$. For later reference, also note that the consequent in Eq. (5.28) is equivalent to

$$P(Y, Z, W|do(X))\; P(W|do(X)) \;=\; P(Y, W|do(X))\; P(Z, W|do(X)) \;. \qquad (5.29)$$

5.6.1.2 Classical processes

Classical strong relative independence from Def. 5.12 has the following generalisation to account for an additional set X, where a do-intervention takes place, such that $(Y \perp\!\!\!\perp Z|W)_{\kappa_{YZW}}$ is recovered for $X = \emptyset$.

Definition 5.16 (Classical strong relative independence with a do-intervention): *Given a classical process κ_{YZWX}, say that Y* and *Z* are *strongly independent relative to $(W,\ do(X))$, and write $(Y \perp\!\!\!\perp Z|W do(X))_{\kappa_{YZWX}}$, if and only if there exist real functions $\alpha_{YWX^{out}} : Y^{in} \times Y^{out} \times W^{in} \times W^{out} \times X^{out} \to \mathbb{R}$ and $\beta_{ZWX^{out}} : Z^{in} \times Z^{out} \times W^{in} \times W^{out} \times X^{out} \to \mathbb{R}$, such that $\kappa_{YZWdo(X)} = \alpha_{YWX^{out}}\ \beta_{ZWX^{out}}$.*

Also Prop. 5.5, which gives an operational statement equivalent to $(Y \perp\!\!\!\perp Z|W)_{\kappa_{YZW}}$, straightforwardly extends to include an additional set X with $do(X)$.

Proposition 5.8 *Given a classical process κ_{YZWX}, then $(Y \perp\!\!\!\perp Z|W do(X))_{\kappa_{YZWX}}$ holds if and only if:*

(COS1) *For all values $X^{out} = x$ of a do-intervention at X, any maximally informative intervention at W with outcome k_W, and any local interventions at Y and Z with outcomes k_Y and k_Z, respectively, the joint probability distribution $P(k_Y, k_Z, k_W)$ satisfies $(k_Y \perp\!\!\!\perp k_Z|k_W)_P$.*

Proof. Observe that the condition $(Y \perp\!\!\!\perp Z|Wdo(X))_{\kappa_{YZWX}}$ is equivalent to the statement that $(Y \perp\!\!\!\perp Z|W)_{\kappa_{YZWdo(X=x)}}$ holds for all values x of a do-intervention at X. The result then follows from Prop. 5.5. □

In order to see that $(Y \perp\!\!\!\perp Z|Wdo(X))_{\kappa_{YZWX}}$ under $I_{\kappa \to P}$ reduces to the consequent of Rule 1, note the observation in the above proof, or alternatively, observe that $(Y \perp\!\!\!\perp Z|Wdo(X))_{\kappa_{YZWX}}$ implies that $\kappa_{YZWdo(X)}\, \kappa_{Wdo(X)} = \kappa_{YWdo(X)}\, \kappa_{ZWdo(X)}$,[10] which under $I_{\kappa \to P}$ reduces to Eq. (5.29).

Given a classical process κ_V, there is no one unique way of calculating the marginal on disjoint subsets $Y, Z, W, X \subseteq V$ (see Sec. 5.5) and the following generalisation of Rule 1 makes the strongest possible statement by quantifying over all possible interventions at the remaining nodes, just as Thm. 5.3 did.

Theorem 5.4 (Rule 1 analogue for classical processes): *Consider a DAG G, with a set V of classical split nodes, and disjoint subsets of nodes Y, Z, W and X, with $R := V \setminus (Y \cup Z \cup W \cup X)$. For any classical process κ_{YZWXR} that is Markov for G,*

$$(Y \perp\!\!\!\perp Z|X, W)_{G_{\overline{X}}} \quad \Rightarrow \quad \forall \tau_R \;\; (Y \perp\!\!\!\perp Z|Wdo(X))_{\kappa^{\tau_R}_{YZWX}}.$$

Proof. The proof is essentially the same as that of Theorem 5.5 below, with classical process maps replacing process operators, classical channels replacing quantum channels, and classical interventions replacing quantum interventions. □

5.6.1.3 Quantum processes

Analogously to the above, quantum strong relative independence can be generalised to allow for a fourth set X, where do-interventions take place, such that $(Y \perp\!\!\!\perp Z|W)_{\sigma_{YZW}}$ is recovered for $X = \emptyset$.

Definition 5.17 (Quantum strong relative independence with a do-intervention): *Given a quantum process σ_{YZWX}, say that Y and Z are strongly independent relative to $(W,\, do(X))$, and write $(Y \perp\!\!\!\perp Z|Wdo(X))_{\sigma_{YZWX}}$, if and only if there exist Hermitian operators $\alpha_{YWX^{out}}$ and $\beta_{ZWX^{out}}$ such that $\sigma_{YZWdo(X)} = \alpha_{YWX^{out}}\, \beta_{ZWX^{out}}$.*

Remark 5.3 *By convention, the appearance of the label of a node, say Y, in the subscript of an operator $\alpha_{YWX^{out}}$ means that it acts on $\mathcal{H}_{Y^{in}} \otimes \mathcal{H}^*_{Y^{out}}$. In order to avoid cluttered notation above and in the remainder of this chapter, when writing $\sigma_{YZWdo(X)} = \alpha_{YWX^{out}}\, \beta_{ZWX^{out}}$ it is understood implicitly that the operators on the right-hand side act on $\mathcal{H}^*_{X^{out}}$, rather than $\mathcal{H}_{X^{out}}$.*

[10] Straightforward calculation, or else, see Prop. 5.10 in conjunction with Rem. 5.5

Also the operational statement implied by $(Y \perp\!\!\!\perp Z|W)_{\sigma_{YZW}}$ from Prop. 5.6 carries over to when allowing for $do(X)$ at some additional nodes X.

Proposition 5.9 *Given a quantum process σ_{YZWX}, if $(Y \perp\!\!\!\perp Z|W do(X))_{\sigma_{YZWX}}$, then:*

(QOS1) *There exists a global intervention at WX^{out}, with outcome $k_{WX^{out}}$, such that for all local interventions at Y, Z, with outcomes k_Y, k_Z respectively, the joint probability distribution $P(k_Y, k_Z, k_{WX^{out}})$, satisfies $(k_Y \perp\!\!\!\perp k_Z|k_{WX^{out}})_P$.*

Proof. See Appendix A.8. □

Remark 5.4 *The global intervention at WX^{out} that yields $(k_Y \perp\!\!\!\perp k_Z|k_{WX^{out}})_P$ for all interventions at Y and Z can be taken to be of the following form: an additional node E is brought in with E^{in} isomorphic to $\mathcal{H}_{W^{in}} \otimes \mathcal{H}_{W^{out}} \otimes \mathcal{H}_{X^{out}}$, then at each node in X the incoming quantum system is ignored, while for each node in W the incoming quantum system is sent to E; for all nodes in W and X, one half of a pair of maximally entangled systems is fed into the output of the node, with the other half sent to E, where finally an appropriate joint von Neumann measurement on E^{in} is performed.*

The set of equivalent statements, which generalises Prop. 5.4, is the following.

Proposition 5.10 *Let σ_{YZWX} be a quantum process over the disjoint sets of nodes Y, Z, W and X. The following statements are equivalent:*

(1) $(Y \perp\!\!\!\perp Z|W do(X))_{\sigma_{YZWX}}$.

(2) $\sigma_{YZW do(X)} \star \sigma^{\tau_Y,\tau_Z}_{W do(X)} = \sigma^{\tau_Z}_{YW do(X)} \star \sigma^{\tau_Y}_{ZW do(X)}$ $\forall$ *local interventions* τ_Y, τ_Z.

(3) $I(Y : Z|WX^{out}) = 0$, *evaluated on* $\hat{\sigma}_{YZW do(X)}$.

Proof. See Appendix A.9. □

Remark 5.5 *Completely analogous statements exist that are equivalent to classical strong relative independence with a do-intervention, $(Y \perp\!\!\!\perp Z|W do(X))_{\kappa_{YZWX}}$. They are obtained from the above by replacing σ_{YZWX} with κ_{YZWX} everywhere, replacing the '$\star$'-product in (2) with ordinary multiplication of functions and $I(Y : Z|WX^{out})$ in (3) with the classical conditional mutual information. The proof is analogous.*

Prop. 5.10 and Rem. 5.5 make evident that $(Y \perp\!\!\!\perp Z|W do(X))_{\sigma_{YZWX}}$ reduces to $(Y \perp\!\!\!\perp Z|W do(X))_{\kappa_{YZWX}}$ under $I_{\sigma\to\kappa}$.

Finally, the quantum analogue of Rule 1, that generalises Thm. 5.4 for classical processes, takes the expected form.

Theorem 5.5 (Analogue of Rule 1 for quantum processes): *Consider a DAG G, with a set V of quantum nodes, and disjoint subsets of nodes Y, Z, W and X, with $R := V \setminus (Y \cup Z \cup W \cup X)$. For any quantum process σ_{YZWXR} that is Markov for G,*

$$(Y \perp\!\!\!\perp Z|X, W)_{G_{\overline{X}}} \quad \Rightarrow \quad \forall \tau_R \;\; (Y \perp\!\!\!\perp Z|W do(X))_{\sigma^{\tau_R}_{YZWX}}.$$

Proof. See App. A.10. □

Soundness of d-separation for quantum strong relative independence (see Thm. 5.3) is the special case of this theorem for $X = \emptyset$. Note that the proof in App. A.10 of the above theorem is not just a straightforward generalisation of the proof technique for the d-separation theorem, thereby actually giving soundness of d-separation for quantum strong relative independence an independent proof.

5.6.1.4 Example

The illustration of the generalisation of Rule 1 will be based on the same DAG G as in Fig. 5.8, which already served to illustrate the d-separation theorem. For convenience, G is shown again below in Fig. 5.9.

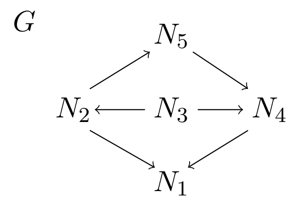


Figure 5.9

Suppose G is the causal structure of the quantum nodes $N_1, \ldots, N_5$ and let $\sigma_{N_1 \ldots N_5}$ be a quantum process that is Markov for G. Now, consider the following two distinct mutilations of G.

$Y = \{N_2\}$ $\quad W = \{N_3, N_5\}$
$Z = \{N_4\}$ $\quad X = \{N_1\}$

(a)

$Y = \{N_2\}$ $\quad W' = \{N_1, N_3\}$
$Z = \{N_4\}$ $\quad X' = \{N_5\}$

(b)

Figure 5.10: For the stated choices of subsets Y, Z, W, X, and X', W', respectively, of the nodes in Fig. 5.9, (a) and (b) depict the mutilated DAGs $G_{\overline{X}}$ and $G_{\overline{X'}}$, where $(Y \perp\!\!\!\perp Z|X, W)_{G_{\overline{X}}}$ holds, while $(Y \perp\!\!\!\perp Z|X', W')_{G_{\overline{X'}}}$ fails.

In G the set $X \cup W$ contains the collider N_1 and therefore does not d-separate Y from Z. However, once arrows into X are taken out then $(Y \perp\!\!\!\perp Z|X, W)_{G_{\overline{X}}}$ holds and, hence, Thm. 5.5 implies $(Y \perp\!\!\!\perp Z|W do(X))_{\sigma_{YZWX}}$. Due to Prop. 5.9, the operational statement (QOS1) then also holds — as expected, considering a do-intervention at the collider cannot underwrite correlations between Y and Z.

In contrast, $(Y \perp\!\!\!\perp Z|X', W')_{G_{\overline{X'}}}$ fails since the collider N_1 is still contained in W'. For the special case of a classical process that is Markov for G, it will generally indeed be the case that the operational statement (COS1) (for the sets Y, Z, W', X') fails — the quantification over all maximally informative interventions not only at N_3, but also N_1, will generally underwrite correlations between Y and Z. Note that the quantum operational statement (QOS1) is much weaker and requires only the existence of one suitable intervention and a do-intervention at N_1 does the job, so that (QOS1) still holds for the sets Y, Z, W', X' even though $(Y \perp\!\!\!\perp Z|W' do(X'))_{\sigma_{YZW'X'}}$ will generally fail.

5.6.2 Generalisation do-calculus rule 2

5.6.2.1 Classical probability distributions

For convenience, Rule 2 is restated here: if the probability distribution $P(...)$ is Markov for the DAG G, then for disjoint sets of nodes Y, Z, X, W it holds that

$$(Y \perp\!\!\!\perp Z|X, W)_{G_{\overline{X}\underline{Z}}} \quad \Rightarrow \quad P(Y|do(X), do(Z), W) = P(Y|do(X), Z, W) \ , \tag{5.30}$$

where, recalling Sec. 3.1.4, $G_{\overline{X}\underline{Z}}$ denotes the DAG obtained from $G_{\overline{X}}$ by additionally removing all arrows coming out of vertices in Z. For later reference, note that the consequent in Eq. (5.30) is equivalent to

$$P(Y,Z,W|do(X))\ P(W|do(X)do(Z)) \\ = P(Y,W|do(X)do(Z))\ P(Z,W|do(X))\ . \quad (5.31)$$

5.6.2.2 Classical processes

The consequent of Rule 2, loosely speaking, says that if knowing W and x for $do(X = x)$, then it does not matter to Y whether one observes $Z = z$ or enforces it via $do(Z = z)$. Translated to the level of split nodes, the intuition is that only what comes out of the Z nodes may matter to the Y nodes. Consider then the following notion for a classical process.

Definition 5.18 (Classical strong independence from broken nodes): *Given a classical process map κ_{YZWX}, say that Y* is strongly independent from Z^{in} relative to (W, $do(X)$, Z^{out})*, and write $(Y \perp\!\!\!\perp Z^{in}|W do(X) Z^{out})_{\kappa_{YZWX}}$, if and only if there exist real functions $\alpha_{YWX^{out}Z^{out}} : Y^{in} \times Y^{out} \times W^{in} \times W^{out} \times X^{out} \times Z^{out} \to \mathbb{R}$ and $\beta_{ZWX^{out}} : Z^{in} \times Z^{out} \times W^{in} \times W^{out} \times X^{out} \to \mathbb{R}$, such that $\kappa_{YZWdo(X)} = \alpha_{YWX^{out}Z^{out}}\ \beta_{ZWX^{out}}$.*

In order to give $(Y \perp\!\!\!\perp Z^{\mathrm{in}}|W do(X) Z^{\mathrm{out}})_{\kappa_{YZWX}}$ an operational reading in the subsequent proposition, we first pin down a special class of classical interventions, which generalise do-interventions and help detect that the 'breaking of Z does not matter to Y'.

Definition 5.19 (Classical breaking intervention): *A* breaking intervention *at a node Z consists of a measurement of Z^{in}, giving outcome k_Z, and the preparation of a fixed value z of Z^{out}. A necessary and sufficient condition is that:*

$$P(k_Z, Z^{out}|Z^{in}) = P(k_Z|Z^{in})\ \delta(Z^{out}, z). \quad (5.32)$$

For Z a set of nodes, a breaking local intervention at Z is a product of breaking interventions at each node in Z.

Proposition 5.11 *Given a classical process κ_{YZWX}, the condition $(Y \perp\!\!\!\perp Z^{in}| W do(X) Z^{out})_{\kappa_{YZWX}}$ holds if and only if:*

(COS2) *For all values $X^{out} = x$ of a do-intervention at X, all maximally informative local interventions at W with outcome k_W, all local interventions at Y with outcome k_Y, and all breaking local interventions at Z with outcome k_Z, the joint probability distribution $P(k_Y, k_Z, k_W)$ satisfies $(k_Y \perp\!\!\!\perp k_Z|k_W)_P$.*

Proof. See Appendix A.11. □

In order to see that $(Y \perp\!\!\!\perp Z^{\text{in}}|Wdo(X)Z^{\text{out}})_{\kappa_{YZWX}}$ reduces to Eq. (5.31) under $I_{\kappa\to P}$, and, hence, also to the consequent of Rule 2, observe that $(Y \perp\!\!\!\perp Z^{\text{in}}|$ $Wdo(X)Z^{\text{out}})_{\kappa_{YZWX}}$ implies that $\kappa_{YZWdo(X)}\ \kappa_{Wdo(X)do(Z)} = \kappa_{ZWdo(X)}\ \kappa_{YWdo(X)do(Z)}$.[11]

We can now state the generalisation of Rule 2.

Theorem 5.6 (Rule 2 analogue for classical processes): *Consider a DAG G, with a set V of classical split nodes, and disjoint subsets of nodes Y, Z, W and X, with $R := V \setminus (Y \cup Z \cup W \cup X)$. For any classical process κ_{YZWXR} that is Markov for G,*

$$(Y \perp\!\!\!\perp Z|X, W)_{G_{\overline{X}\underline{Z}}} \quad \Rightarrow \quad \forall \tau_R \ \ (Y \perp\!\!\!\perp Z^{in}|Wdo(X)Z^{out})_{\kappa^{\tau_R}_{YZWX}}.$$

Proof. The proof is essentially the same as that of Thm. 5.7 below, with classical process maps replacing process operators, classical channels replacing quantum channels, and classical interventions replacing quantum interventions. □

5.6.2.3 Quantum processes

The immediate quantum analogue to Def. 5.18 is the following.

Definition 5.20 (Quantum strong independence from broken nodes): *Given a quantum process σ_{YZWX}, say that Y* is strongly independent from Z^{in}, relative to $(W$, $do(X)$, $Z^{\text{out}})$*, and write $(Y \perp\!\!\!\perp Z^{in}|Wdo(X)Z^{out})_{\sigma_{YZWX}}$, if and only if there exist Hermitian operators $\alpha_{YWX^{out}Z^{out}}$ and $\beta_{ZWX^{out}}$ such that $\sigma_{YZWdo(X)} = \alpha_{YWX^{out}Z^{out}}$ $\beta_{ZWX^{out}}$.*

The condition $(Y \perp\!\!\!\perp Z^{\text{in}}|Wdo(X)Z^{\text{out}})_{\sigma_{YZWX}}$ has an implied operational statement, similar in spirit to the one for classical processes in Prop. 5.11, but, as always, modulo that there is no quantum analogue of a maximally informative intervention at the W nodes.

Proposition 5.12 *Given a quantum process σ_{YZWX}, if it holds that $(Y \perp\!\!\!\perp Z^{in}|$ $Wdo(X)Z^{out})_{\sigma_{YZWX}}$, then:*

(QOS2) *There exists a global intervention at $WX^{out}Z^{out}$, with outcome $k_{WX^{out}Z^{out}}$, such that for all interventions at Y, with outcome k_Y, and all measurements of Z^{in} with outcome $k_{Z^{in}}$, the joint probability distribution $P(k_Y, k_{Z^{in}}, k_{WX^{out}Z^{out}})$ satisfies $(k_Y \perp\!\!\!\perp k_{Z^{in}}|k_{WX^{out}Z^{out}})_P$.*

Proof. See Appendix A.12. □

[11] Straightforward calculation, or else, see Prop. 5.13 in conjunction with Rem. 5.7

Remark 5.6 *The required global intervention at $WX^{out}Z^{out}$ that yields $(k_Y \perp\!\!\!\perp k_{Z^{in}}| k_{WX^{out}Z^{out}})_P$ for all interventions at Y and all measurements of Z^{in} can be taken to be basically the same as in Rem. 5.4, apart from additionally feeding one half of a pair of maximally entangled systems into Z^{out} with the other half sent to E.*

Also for $(Y \perp\!\!\!\perp Z^{\text{in}}|W do(X) Z^{\text{out}})_{\sigma_{YZWX}}$, there exists a set of equivalent statements, similar in form to those in Prop. 5.10.

Proposition 5.13 *Given a quantum process σ_{YZWX}, the following statements are equivalent:*

(1) $(Y \perp\!\!\!\perp Z^{in}|W do(X) Z^{out})_{\sigma_{YZWX}}$.

(2) $\sigma_{YZWdo(X)} \star \sigma^{\tau_Y}_{Wdo(X)do(Z)} = \sigma^{\tau_Y}_{ZWdo(X)} \star \sigma_{YWdo(X)do(Z)}$ $\forall$ *local interventions* τ_Y.

(3) $I(Y : Z^{in}|WX^{out}Z^{out}) = 0$, *evaluated on* $\hat{\sigma}_{YZWdo(X)}$.

Proof. See Appendix A.13. □

Remark 5.7 *Completely analogous statements exist that are equivalent to $(Y \perp\!\!\!\perp Z^{in}|W do(X) Z^{out})_{\kappa_{YZWX}}$ in case of classical processes, by replacing σ_{YZWX} with κ_{YZWX} everywhere, replacing the '$\star$'-product in (2) with ordinary multiplication of functions and $I(Y : Z^{in}|WX^{out}Z^{out})$ in (3) with the classical conditional mutual information. The proof is analogous.*

Prop. 5.13 and Rem. 5.7 make evident that $(Y \perp\!\!\!\perp Z^{\text{in}}|W do(X) Z^{\text{out}})_{\sigma_{YZWX}}$ reduces to $(Y \perp\!\!\!\perp Z^{\text{in}}|W do(X) Z^{\text{out}})_{\kappa_{YZWX}}$ under $I_{\sigma\to\kappa}$.

The quantum analogue of Rule 2 can now be stated as follows.

Theorem 5.7 (Rule 2 analogue for quantum processes): *Consider a DAG G, with a set V of quantum nodes, and disjoint subsets of nodes Y, Z, W and X, with $R := V \setminus (Y \cup Z \cup W \cup X)$. For any quantum process σ_{YZWXR} that is Markov for G, it holds that*

$$(Y \perp\!\!\!\perp Z|X, W)_{G_{\overline{X}\underline{Z}}} \quad \Rightarrow \quad \forall \tau_R \;\; (Y \perp\!\!\!\perp Z^{in}|W do(X) Z^{out})_{\sigma^{\tau_R}_{YZWX}}.$$

Proof. See Appendix A.14. □

5.6.2.4 Example

The illustration of the generalisation of Rule 2 will again be based on the same DAG G as in Fig. 5.9, reproduced here in Fig. 5.11.

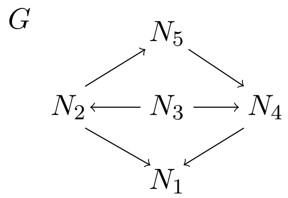


Figure 5.11

Suppose G is the causal structure of the quantum nodes $N_1, \ldots, N_5$ and let $\sigma_{N_1 \ldots N_5}$ be a quantum process that is Markov for G. Now, consider the following two distinct mutilations of G.

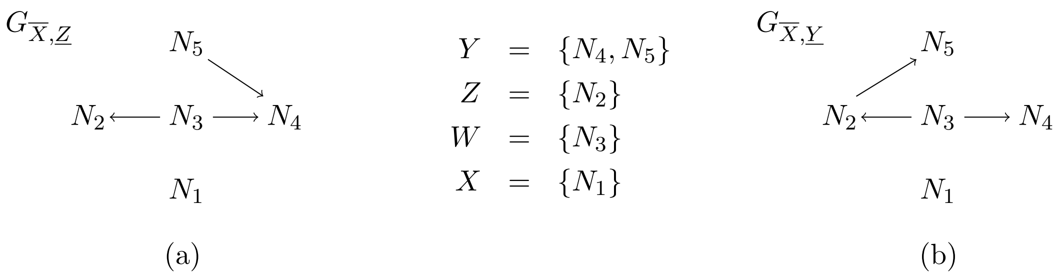


Figure 5.12: For the stated choices of subsets Y, Z, W, X of the nodes in Fig. 5.11, (a) and (b) depict the mutilated DAGs $G_{\overline{X},\underline{Z}}$ and $G_{\overline{X},\underline{Y}}$, where $(Y \perp\!\!\!\perp Z|X, W)_{G_{\overline{X},\underline{Z}}}$ holds, while $(Z \perp\!\!\!\perp Y|X, W)_{G_{\overline{X},\underline{Y}}}$ fails.

Common to both, $G_{\overline{X},\underline{Z}}$ and $G_{\overline{X},\underline{Y}}$, is that the arrows into X were taken out, reflecting that here we will only consider do-interventions at the collider in X. Unlike the considered subsets of nodes in Sec. 5.6.1.4, now N_5 is contained in Y. Hence, there is a direct causal pathway from Z to Y and these two sets are not d-separated by $X \cup W$ in $G_{\overline{X}}$ — interventions at Y and Z will typically not be independent conditional on the outcome of any intervention at W.

However, if considering a special intervention at Z, that just measures Z^{in} and prepares some fixed state independent from $k_{Z^{\text{in}}}$, then the outcome at Y would be expected to be independent from $k_{Z^{\text{in}}}$, at least conditional on the outcome of an appropriate intervention at W, the common cause to Y and Z. For such special interventions at Z it is therefore enough to check a corresponding d-separation condition in the further mutilated graph once arrows coming out of Z are taken out, too. Indeed, $(Y \perp\!\!\!\perp Z|X,W)_{G_{\overline{X},\underline{Z}}}$ holds and Thm. 5.7 therefore implies $(Y \perp\!\!\!\perp Z^{\mathrm{in}}|W do(X) Z^{\mathrm{out}})$, and thus by Prop. 5.12 the operational statement (QOS2) holds.

In contrast, if one considered such a 'breaking' intervention at Y, obviously no independence between the outcomes at Y and Z would be expected to hold, because the input space at N_5 will have direct causal influence from Z. This is captured by the fact that $(Z \perp\!\!\!\perp Y|X,W)_{G_{\overline{X},\underline{Y}}}$ fails.

5.6.3 Generalisation do-calculus rule 3

5.6.3.1 Classical probability distributions

For convenience, Rule 3 is restated here: if the probability distribution $P(...)$ is Markov for the DAG G, then for disjoint sets of nodes Y, Z, X, W it holds that

$$(Y \perp\!\!\!\perp Z|X,W)_{G_{\overline{X},\overline{Z(W)}}} \quad \Rightarrow \quad P(Y|do(X),do(Z),W) = P(Y|do(X),W) \ , \quad (5.33)$$

where, recalling Sec. 3.1.4, $Z(W)$ denotes the subset of all those vertices in Z that are not ancestors of W in $G_{\overline{X}}$. For later reference, note that the consequent in Eq. (5.33) is equivalent to

$$P(Y,W|do(X)do(Z)) \ P(W|do(X)) = P(Y,W|do(X)) \ P(W|do(X)do(Z)). \quad (5.34)$$

5.6.3.2 Classical processes

The consequent in Eq. (5.33), loosely speaking, says that if knowing W and x for $do(X = x)$, then whether or not an intervention takes place at Z makes no difference to Y. Consider the following analogous notion for classical processes, which appears slightly involved, but has a simple operational meaning as expressed in the subsequent proposition.

Definition 5.21 (Classical strong independence from settings): *Given a classical process κ_{YZWX}, say that* Y is strongly independent from the setting at Z, relative to $(W,\, do(X))$, *and write $(Y \perp\!\!\!\perp Set(Z)|W do(X))_{\kappa_{YZWX}}$, if and only if there is a real-valued function $\eta_{YWX^{out}} : Y^{in} \times Y^{out} \times W^{in} \times W^{out} \times X^{out} \to \mathbb{R}$ such that for all local interventions τ_Z at Z, there is a real valued function $\xi^{\tau_Z}_{WX^{out}} : W^{in} \times W^{out} \times X^{out} \to \mathbb{R}$, such that*

$$\kappa^{\tau_Z}_{YW do(X)} \ = \ \eta_{YWX^{out}} \ \xi^{\tau_Z}_{WX^{out}}.$$

Proposition 5.14 *Given a classical process κ_{YZWX}, the condition $(Y \perp\!\!\!\perp Set(Z)|$ $W do(X))_{\kappa_{YZWX}}$ holds if and only if:*

(COS3) *For all values $X^{out} = x$ of a do-intervention at X, all maximally informative local interventions at W with outcome k_W, and all local interventions at Y with outcome k_Y, the conditional probability $P(k_Y|k_W)$ is independent of the choice of local intervention at Z.*

Proof. See Appendix A.15. □

In order to see that $(Y \perp\!\!\!\perp Set(Z)|Wdo(X))_{\kappa_{YZWX}}$ under $I_{\kappa\to P}$ reduces to Eq. (5.34), and, hence, to the consequent of Rule 3, observe that if $(Y \perp\!\!\!\perp Set(Z)|Wdo(X))_{\kappa_{YZWX}}$, then for all z:

$$\begin{aligned}
\kappa^{do(Z=z)}_{YWdo(X)}\ \kappa_{Wdo(X)} &= \left(\eta_{YWX^{\text{out}}}\ \xi^{do(Z=z)}_{WX^{\text{out}}}\right)\left(\sum_Y \left(\eta_{YWX^{\text{out}}}\ \tau^{\text{id}}_Y\right)\ \xi^{\tau^{\text{id}}_Z}_{WX^{\text{out}}}\right)\\
&= \left(\sum_Y \left(\eta_{YWX^{\text{out}}}\ \tau^{\text{id}}_Y\right)\ \xi^{do(Z=z)}_{WX^{\text{out}}}\right)\left(\eta_{YWX^{\text{out}}}\ \xi^{\tau^{\text{id}}_Z}_{WX^{\text{out}}}\right)\\
&= \kappa^{do(Z=z)}_{Wdo(X)}\ \kappa_{YWdo(X)}\ .
\end{aligned}$$

We can now state the generalisation of Rule 3 as follows.

Theorem 5.8 (Rule 3 analogue for classical processes): *Consider a DAG G, with a set V of classical split nodes, and disjoint subsets of nodes Y, Z, W and X, with $R := V \setminus (Y \cup Z \cup W \cup X)$. For any classical process κ_{YZWXR} that is Markov for G,*

$$(Y \perp\!\!\!\perp Z|X,W)_{G_{\overline{X},\overline{Z(W)}}} \quad\Rightarrow\quad \forall \tau_R\ \ (Y \perp\!\!\!\perp Set(Z)|Wdo(X))_{\kappa^{\tau_R}_{YZWX}}.$$

Proof. The proof is essentially the same as that of Thm. 5.9 below, with classical process maps replacing process operators, classical channels replacing quantum channels, and classical interventions replacing quantum interventions. □

5.6.3.3 Quantum processes

Finally, the immediate quantum analogue to Def. 5.21 is the following.

Definition 5.22 (Quantum strong independence from settings): *Given a quantum process σ_{YZWX}, say that Y* is strongly independent from the setting at Z, relative to $(W,\ do(X))$, *and write $(Y \perp\!\!\!\perp Set(Z)|Wdo(X))_{\sigma_{YZWX}}$, if and only if there is a Hermitian operator $\eta_{YWX^{out}}$ such that for all local interventions τ_Z at Z, there is a Hermitian operator $\xi^{\tau_Z}_{WX^{out}}$, such that*

$$\sigma^{\tau_Z}_{YWdo(X)} \;=\; \eta_{YWX^{out}}\ \xi^{\tau_Z}_{WX^{out}}\ .$$

Again, there is the expected operational statement, analogous to (COS3), that is implied by $(Y \perp\!\!\!\perp Set(Z)|Wdo(X))_{\sigma_{YZWX}}$.

Proposition 5.15 *Given a quantum process σ_{YZWX}, if it holds that $(Y \perp\!\!\!\perp Set(Z)| Wdo(X))_{\sigma_{YZWX}}$, then:*

(QOS3) *There exists a global intervention at WX^{out}, with outcome $k_{WX^{out}}$, such that for all local interventions at Y, with outcome k_Y, the conditional probability $P(k_Y|k_{WX^{out}})$ is independent of the choice of local intervention at Z.*

Proof. See App. A.16. □

Remark 5.8 *The global intervention at WX^{out} that yields the independence of $P(k_Y|k_{WX^{out}})$ from the choice of local intervention at Z for all local interventions at Y can be taken to be the same as the one described in Rem. 5.4.*

In contrast to the generalisations of Rule 1 and Rule 2, there are no statements equivalent to $(Y \perp\!\!\!\perp Set(Z)|Wdo(X))_{\sigma_{YZWX}}$, which are of an analogous form to those in Prop. 5.10 and Prop. 5.13. Note that $(Y \perp\!\!\!\perp Set(Z)|Wdo(X))_{\sigma_{YZWX}}$ reduces to $(Y \perp\!\!\!\perp Set(Z)|Wdo(X))_{\kappa_{YZWX}}$ under $I_{\sigma\to\kappa}$.[12]

The quantum analogue of Rule 3 can now be stated as follows.

Theorem 5.9 (Rule 3 analogue for quantum processes): *Consider a DAG G, with a set V of quantum nodes, and disjoint subsets of nodes Y, Z, W and X, with $R := V \setminus (Y \cup Z \cup W \cup X)$. For any quantum process σ_{YZWXR} that is Markov for G, it holds that*

$$(Y \perp\!\!\!\perp Z|X,W)_{G_{\overline{X},\overline{Z(W)}}} \quad \Rightarrow \quad \forall \tau_R \ \ (Y \perp\!\!\!\perp Set(Z)|Wdo(X))_{\sigma^{\tau_R}_{YZWX}} \ .$$

Proof. See App. A.17. □

5.6.3.4 Example

The illustration of the generalisation of Rule 3 will again be based on the same DAG G as for Rule 1 and Rule 2, which is reproduced here in Fig. 5.13.

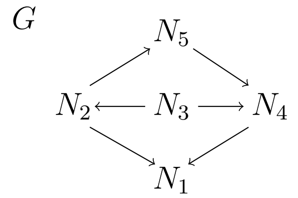


Figure 5.13

[12]In order to see that under $I_{\sigma\to\kappa}$ for each τ_Z, the operators $\eta_{YWX^{\text{out}}}$ and $\xi^{\tau_Z}_{WX^{\text{out}}}$ can be chosen to be diagonal in the same basis in which $\sigma^{\tau_Z}_{YWdo(X)}$ is diagonal (only non-obvious in case of degenerate eigenbases), observe that this is immediate from the block-diagonal structure of $\eta_{YWX^{\text{out}}}\xi^{\tau_Z}_{WX^{\text{out}}}$ that is used in the proof of Prop. 5.15.

Suppose G is the causal structure of the quantum nodes $N_1, \ldots, N_5$ and let $\sigma_{N_1 \ldots N_5}$ be a quantum process that is Markov for G. Now, consider the following two distinct mutilations of G.

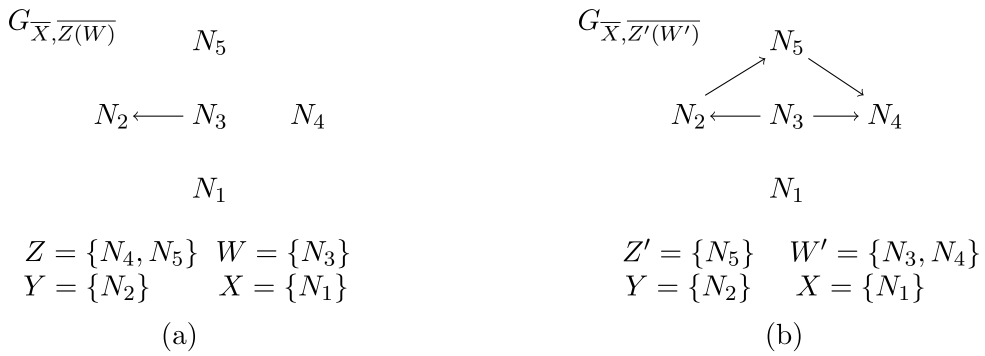


Figure 5.14: For the stated choices of subsets Y, Z, W, X and Z', W', respectively, of the nodes in Fig. 5.13, (a) and (b) depict the mutilated DAGs $G_{\overline{X},\overline{Z(W)}}$ and $G_{\overline{X},\overline{Z'(W')}}$, where $(Y \perp\!\!\!\perp Z|X, W)_{G_{\overline{X},\overline{Z(W)}}}$ holds, while $(Y \perp\!\!\!\perp Z'|X, W')_{G_{\overline{X},\overline{Z'(W')}}}$ fails.

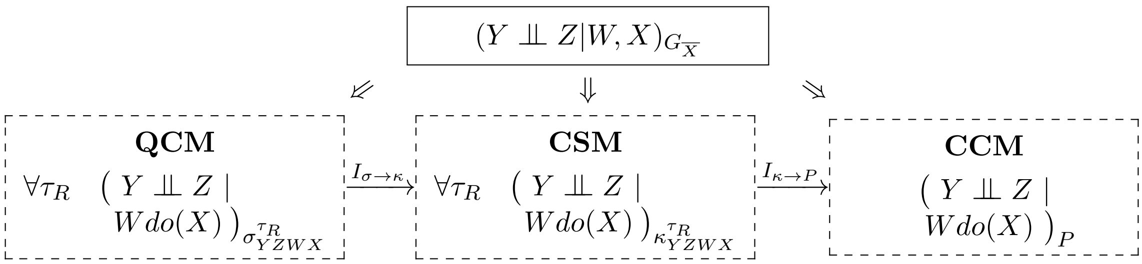
The two mutilated DAGs again share that the arrows into X have been taken out, since at X only do-interventions will be considered in the following.

There is no direct causal pathway from Z to Y in G and there are no ancestors of W in Z (i.e. $Z = Z(W)$). It holds that $(Y \perp\!\!\!\perp Z|X, W)_{G_{\overline{X},\overline{Z(W)}}}$, thus, Thm. 5.9 implies $(Y \perp\!\!\!\perp Set(Z)|W do(X))_{\sigma_{YZWX}}$ and, hence, Prop. 5.15 implies the operational statement (QOS3). This is as expected, because choosing different interventions at Z could not directly influence Y and there is no 'inferential link' via some collider. In this case, because of the simplicity of the example, the distribution $P(k_Y|\tau_Z)$ will be independent from the choice of intervention τ_Z at the Z nodes, no matter what intervention at W is performed (i.e. no matter which state at N_3 is prepared), provided a do-intervention at X.

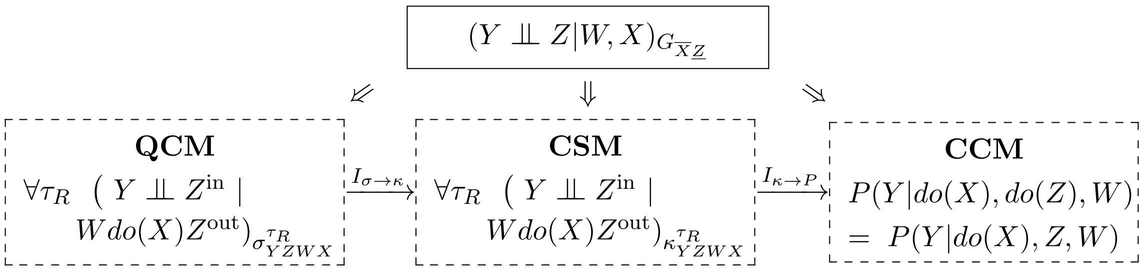
In contrast, even though there still is no direct causal pathway from Z' to Y, now that N_4 is included in W', then Z' does have ancestors in W' (in fact, $Z'(W') = \emptyset$) and $(Y \perp\!\!\!\perp Z'|X, W')_{G_{\overline{X},\overline{Z'(W')}}}$ fails. Consider for simplicity a classical process $\kappa_{YZ'W'X}$. Now, in the specific case of Fig. 5.14b the presence of a fork at N_3 on the path from Z' to Y actually still prevents signalling from Z' to Y once conditioned on the outcome of maximally informative interventions at W'. The simple DAG in Fig. 5.13 just does not allow to give a simple example where $(Y \perp\!\!\!\perp Z'|X, W')_{G_{\overline{X},\overline{Z'(W')}}}$ fails and also $(Y \perp\!\!\!\perp Set(Z')|W' do(X))_{\kappa_{YZ'W'X}}$ fails. However, the intuition behind the graphical antecedent in Thm. 5.8 is clear – if W'

contains a collider then conditioning on the outcome of maximally informative interventions at W' can in general underwrite correlations so that one may signal to Y through choosing an intervention at Z'.

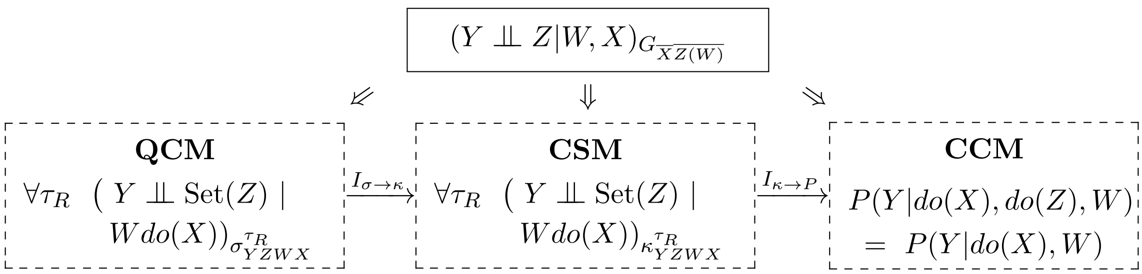
5.6.4 Overview



(a) Generalisation of Rule 1.



(b) Generalisation of Rule 2.



(c) Generalisation of Rule 3.

Figure 5.15: Overview of all three rules for classical causal models from Thm. 3.3, together with their respective generalisations for classical split-node causal models and quantum causal models.

5.7 From causation to signalling and back

The preceding sections of this chapter have a common feature, namely, what the given is in the respective questions that are being asked. They all are of the form: given causal structure, as defined in Chap. 4, what are its ramifications for quantum processes? This question led to the definition of a quantum causal model and the results so far can then be seen to establish Def. 5.1 as the appropriate definition of a quantum causal model. This conclusion stems in particular from the equivalence result from Section 5.2.3, with further support coming from the fact that this framework allows for the generalisation of the d-separation theorem in Sec. 5.5 and of the three rules of the classical do-calculus in Sec. 5.6.

Having thus built confidence in the definition, the direction of the question should be turned around: given a quantum process $\sigma_{A_1 \dots A_n}$, what can we say about causal structure? This leads to the formulation of a problem of quantum causal inference, which a framework of quantum causal models had better be able to say something about. The following will make a start with this direction of inquiry. This requires first spelling out the relation between causation and 'signalling relations', the latter being the central empirically accessible concept for generic quantum processes.

At the formal level it makes no difference whatsoever to the following exposition whether one allows for arbitrary quantum nodes or not. In the view that causal relata should be considered quantum $\imath$nodes — thinking of causal reasoning as one about quantum systems without a need for an intervention — one may also see the following in this light (see Sec. 3.2.5.2 and 4.2). However, for the sake of generality and in order not to impose any philosophical ladenness, the restriction to quantum $\imath$nodes from Secs. 5.3-5.6 is henceforth dropped again in the rest of the thesis.

5.7.1 Signalling and processes

The notion of 'signalling' is an interventionist one that involves the notion of agents who act as senders and receivers. Given a quantum process $\sigma_{A_1 \dots A_n}$ the quantum nodes $A_1, \dots, A_n$ are in particular loci of intervention, where one may imagine an agent to be stationed and able to perform arbitrary quantum instruments. Sec. 3.2.3 introduced in Def. 3.8, what it means, given a quantum process σ_{STR} with disjoint sets of nodes S, T, R, that *the nodes S cannot signal to the nodes T*, written $(S \not\to^s T)_{\sigma_{STR}}$. Then say the *nodes S can signal to the nodes T*, write $(S \to^s T)_{\sigma_{STR}}$, if and only if $\neg(S \not\to^s T)_{\sigma_{STR}}$, i.e. there exists an intervention $\tau_T^{k_T}$ and interventions τ_R such that $p(k_T|\tau_S) \neq p(k_T|\tau'_S)$ for at least a pair of interventions τ_S, τ'_S.

By just considering pairs of individual nodes, rather than pairs of sets of nodes, this notion induces a directed graph.

Definition 5.23 (Induced signalling directed graph): *Given a quantum process $\sigma_{A_1 \dots A_n}$, let the* induced signalling directed graph *be the directed graph with vertices $\{A_1, \dots, A_n\}$ and an arrow $A_i \to A_j$ whenever $(A_i \to^s A_j)_{\sigma_{A_1 \dots A_n}}$.*

Importantly, a quantum process' induced signalling directed graph is in general an *incomplete representation* of a process' signalling relations: even though there may not be signalling from A_i to A_j and also not from A_i to A_k for $i \neq j \neq k$, there may be signalling from A_i to the set of nodes $\{A_j, A_k\}$, while a complete representation has to capture the set of signalling relations between all pairs of disjoint subsets of nodes. Nonetheless, the induced signalling directed graph is arguably the most complete *directed* graph, associated with the signalling relations in a quantum process, rather than, say, a hypergraph — hence the name 'induced signalling directed graph' despite the limited information it conveys.

Also note that, given the generality of the process formalism, a quantum process' induced signalling directed graph is generally not a DAG. However, this chapter is not concerned with the study of those cases, where it is not a DAG. A corresponding discussion is postponed to Chap. 7.

Now recall that any quantum process $\sigma_{A_1 \dots A_n}$ also defines a channel $\mathcal{P}$ from the output spaces of all nodes to their input spaces via $\sigma_{A_1 \dots A_n} = \rho^{\mathcal{P}}_{A_1 \dots A_n | A_1 \dots A_n}$. As such, one can study the relations of (no-)signalling according to Def. 3.6 from any set of A_j^{out} — the input systems of $\mathcal{P}$ — to any set of A_i^{in} — the output systems of $\mathcal{P}$. Consider the directed graph that arises based on that by associating both A_i^{out} and A_i^{in} with one vertex, to represent the quantum nodes $A_1, \dots, A_n$, as follows.

Definition 5.24 (Induced direct-signalling directed graph): *Given a process operator $\sigma_{A_1 \dots A_n}$, let its* induced direct-signalling directed graph, *denoted G_σ, be the one defined by the associated channel $\rho^{\mathcal{P}}_{A_1 \dots A_n | A_1 \dots A_n}$ as follows: it has vertices $A_1, \dots, A_n$ and an arrow $A_i \to A_j$ whenever A_i^{out} can signal to A_j^{in} through the channel $\mathcal{P}$, i.e. $\neg(A_i^{out} \not\to^s A_j^{in})$.*

Importantly, G_σ is in general again an *incomplete representation* of, now the direct signalling relations between nodes. This is for the same reason as ever, discussed in Secs. 3.2.4 and 4.1, namely, that the set of no-signalling relations for individual output systems of a channel does not in general determine the no-signalling relations for sets of output systems.

It is easy to see that G_σ is a subgraph of the induced signalling directed graph from Def. 5.23. In fact, G_σ can alternatively be characterised as the subgraph obtained by drawing an arrow from A_i to A_j if there is signalling from A_i to A_j when quantifying over only do-interventions at A_i and the remaining nodes, rather than arbitrary interventions as in Def. 3.8. This is the reason the signalling relations of this kind are referred to as direct signalling, seeing as it is not mediated through other nodes — the do-interventions break the influence. Consider for instance the simple situation of $\sigma_{ABC} = \rho_{C|B}\ \rho_{B|A}\ \rho_A$, where all input and output spaces are qubits and $\rho_{C|B}$ and $\rho_{B|A}$ are two unitary channels. The process' graph G_σ is the chain $A \to B \to C$, while in the induced signalling directed graph according to Def. 5.23, there would be an arrow from A to C, too. The latter signalling relation is however only mediated through B and hence not regarded as direct signalling.

The bottom line is that also G_σ is generally not a DAG and that an arrow in G_σ has the obvious meaning — there is signalling between the respective nodes — while absences of arrows in G_σ are inconclusive — both with respect to *direct* signalling between *sets* of nodes and *indirect* signalling between *individual* nodes, as well as the combination of the two kinds.

5.7.2 Signalling and the Markov condition

Suppose the quantum process $\sigma_{A_1 \ldots A_n}$ is Markov for the DAG G and therefore factorises accordingly into pairwise commuting operators $\sigma_{A_1 \ldots A_n} = \prod_i \rho_{A_i|Pa(A_i)}$. There are then some immediate observations regarding the signalling properties of $\sigma_{A_1 \ldots A_n}$.

First, the marginal channel $\rho_{A_i|Pa(A_i)}$ allows signalling to A_i^{in} from the output systems of at most those nodes that are contained in $Pa(A_i)$. Hence, by Def. 5.24, the induced direct-signalling directed graph G_σ necessarily is a subgraph of G. In particular, G_σ is also a DAG and G has to contain all arrows G_σ has.

Second, by our convention of suppressing identity operators, it also holds that $\sigma_{A_1 \ldots A_n} = \prod_i \rho_{A_i|Pa^{G_\sigma}(A_i)}$, where the parental sets refer to G_σ, that is, the process $\sigma_{A_1 \ldots A_n}$ is also Markov for G_σ.

Third, since the marginal channel into $A_j^{\text{in}} A_k^{\text{in}}$ is given by $\rho_{A_j|Pa^{G_\sigma}(A_j)} \rho_{A_k|Pa^{G_\sigma}(A_k)}$, it holds that if A_i^{out} cannot signal to A_j^{in} and also not to A_k^{in}, then it cannot signal to the composite $A_j^{\text{in}} A_k^{\text{in}}$ either [13] . Hence, the DAG G_σ is a complete representation of the direct signalling relations between the nodes of $\sigma_{A_1 \ldots A_n}$.

Fourth, in the converse direction, adding further arrows to G, instead of taking arrows out, does not destroy the Markov property for the new DAG if appropriately padding $\rho_{A_i|Pa^{G_\sigma}(A_i)}$ with identity operators.

[13] This is the same argument as for the analogous property for causal influence in a unitary channel in Sec. 4.1, the crucial difference being that for the latter it is enforced by unitarity due to Thm. 4.1, while for the channel defining a generic process the Markov condition is a non-trivial condition to hold.

In summary:

Remark 5.9 *Given a quantum process $\sigma_{A_1...A_n}$, if it is Markov for some DAG G, then it is also Markov for G_σ, and conversely, if it is Markov for G_σ it is Markov for any DAG with the same vertices that contains G_σ as a subgraph. One may therefore also speak of a quantum process being Markov or not, independently from which particular DAG.*

A pair $(G, \sigma_{A_1...A_n})$, where $\sigma_{A_1...A_n}$ is Markov for the DAG G is a quantum causal model. What then is the status of all those DAGs with 'extraneous' arrows compared to G_σ, for which the process is Markov and which, together with $\sigma_{A_1...A_n}$, all form QCMs?

Suppose $(G, \sigma_{A_1...A_n})$ is a QCM and that there is an arrow from A_i to A_j in G that is absent in G_σ. It may well be the case that there is direct causal influence from node A_i to node A_j in the actual underlying unitary process, hence the corresponding arrow in G; however, due to some particular state ρ_λ for some latent root node, for which $\sigma_{A_1...A_n}$ is recovered from the unitary process, the direct signalling from A_i^{out} to A_j^{in} disappears in the effective description with $\sigma_{A_1...A_n}$. The underlying causal mechanism is still present and would allow for signalling in case of a different state ρ_λ, which is not *'fine-tuned'* to make the signalling from A_i to A_j disappear. Such QCMs are perfectly conceivable and in fact an important part of the framework — a relation of direct signalling is a sufficient but not a necessary condition for the presence of a causal relation.

Call a quantum causal model $(G, \sigma_{A_1...A_n})$ *faithful*[14] if and only if there are no 'extraneous' arrows in the DAG G that do not correspond to direct signalling relations, i.e. if it holds that $G = G_\sigma$. A QCM is called non-faithful otherwise. This borrows terminology from classical causal models (see Sec. 3.1.3), where a faithful classical causal model $(G, P(X_1, \ldots, X_n))$ is one, where there is no extraneous conditional independence relation that the probability distribution $P(X_1, \ldots, X_n)$ satisfies, but that is not enforced by a corresponding d-separation relation in the causal structure G (see Thm. 3.2).

Remark 5.10 *Note that at the end of Sec. 5.2.3 it was left open whether the equivalence between Markovianity and compatibility can also be proven to hold for a stronger version of compatibility with a DAG G that requires all arrows of G to correspond to causal influence in the asserted underlying unitary process, rather than merely requiring the unitary process to satisfy the no-influence relations according*

[14]Also in Ref. [82] this terminology was used for the same concept, only based on the corresponding definition of a QCM from Ref. [82].

to G. Suppose $(G, \sigma_{A_1 \dots A_n})$ is a faithful quantum causal model, that is $G = G_\sigma$. In that case the two notions of compatibility coincide, since the unitary process asserted to exist by compatibility via Thm. 5.2 necessarily has to allow all ways of causal influence corresponding to G_σ — signalling can disappear, but not appear when marginalising over root and leaf nodes. Arguably, this is the most important case anyway, but for all other non-faithful quantum causal models the question from Sec. 5.2.3 concerning the stronger notion of compatibility remains open.

5.7.3 Quantum causal inference

Traditionally, the problem of causal inference[15] is *the* problem that motivated the development of a causal model framework, so that it could be addressed scientifically: given a probability distribution that encodes purely observational data, how can one infer the causal structure between the variables in a principled way, that is, under which additional assumptions? As mentioned in Sec. 3.1.3 the seminal causal discovery algorithms of the classical causal model framework answer the question for many situations (see, e.g., Refs. [8, 9]).

In the quantum case, the same problem obviously does not exist, because there is no object that encodes 'purely observational quantum data' and that would bear the same kind of ambiguity as a probability distribution does, when it comes to giving causal explanations. First works on inferring the causal relation between two quantum systems given data on outcomes of measurements on those systems can be found in, e.g., Refs. [79, 81]. Generally, the empirical object, with which any set of quantum systems can be described, and in terms of which the constraints from causal structure are most elegantly stated, is a quantum process operator. As such, it already allows predictions for arbitrary interventions. Conversely, one needs informationally complete sets of interventions at all nodes to obtain a process operator experimentally. Causal discovery problems given a process operator may therefore not be considered a particularly relevant problem, practically speaking. It would be interesting to see whether there is a 'more practically relevant' problem that asks about causal explanations, when the given data only leads to an incomplete knowledge of the quantum process, and where the data is of the sort that may be available in typical situations in laboratories or future quantum information processing set-ups.

Nonetheless, given a quantum process $\sigma_{A_1 \dots A_n}$, there are essential questions, precisely of a causal nature, and being able to answer them is not only of foundational

[15]Causal inference and causal discovery are used synonymously here.

interest but also the very basis for potential, more practically relevant, future versions of causal discovery:

(1) Is $\sigma_{A_1 \ldots A_n}$ compatible at all with a causal order of the quantum nodes?

(2) If so, what is a plausible causal explanation of $\sigma_{A_1 \ldots A_n}$ within the framework of quantum causal models?

A first step in answering such questions in a principled way was taken by Costa and Shrapnel in Ref. [82] and a further step by Giarmatzi and Costa in Ref. [121], where a detailed quantum causal discovery algorithm was presented, based on the definition of a quantum causal model from Ref. [82] (see Sec. 3.2.4 for that approach). Inspired by the work in Ref. [121], the following will sketch similar steps, albeit in much less detail, adjusted to the more general definition of a quantum causal model in this work. One other main difference is that the input data to the algorithm from Ref. [121] includes a specification of the factorisation of each node's output space into subsystems. It is these subsystems that are then considered as the potential systems that mediate the causal influence along the causal arrows of the to-be-discovered DAG, owing to the notion of a quantum causal model from Ref. [82]. The input data thus already includes substantial causal knowledge, namely, how many children a node may have at most and which subsystems may play the role of another node's direct cause.

The classical causal discovery algorithms have at their heart, amongst other assumptions like faithfulness or the absence of latent common causes, the idea of putting the *causal principle* to work: if a given probability distribution $P(X_1, \ldots, X_n)$ is *not* Markov for a DAG G with vertices $X_1, \ldots, X_n$, then G is *not* a plausible causal explanation of P. In the quantum case, the idea equally is to put the *quantum causal principle* from Sec. 5.1 to work: if a quantum process $\sigma_{A_1 \ldots A_n}$ is *not* Markov for the DAG G then G is *not* a plausible causal explanation of $\sigma_{A_1 \ldots A_n}$. Building on the observations from the Sec. 5.7.2, this is now straightforward.

A simple version of a quantum causal discovery algorithm, which takes a quantum process operator $\sigma_{A_1 \ldots A_n}$ as its input, does the following. It first calculates G_σ, that is, the parental sets $\{Pa(A_i)\}_{i=1}^n$ by checking the corresponding $n(n-1)$ linear constraints:

$$A_j \notin Pa(A_i) \quad \textit{iff} \quad \frac{1}{d_{A_j^{out}}} \mathrm{Tr}_{(A_j^{out})^*}\left[\rho_{A_i|A_1 \ldots A_n}\right] \otimes \mathbb{1}_{(A_j^{out})^*} \;=\; \rho_{A_i|A_1 \ldots A_n} \;, \tag{5.35}$$

where $\rho_{A_i|A_1 \ldots A_n} := \mathrm{Tr}_{A_k^{in}, \forall k, k \neq i}\left[\sigma_{A_1 \ldots A_n}\right]$. The algorithm then checks whether G_σ is a DAG, and in case it is, the algorithm then checks whether $\sigma_{A_1 \ldots A_n}$ is Markov for

G_σ and outputs the findings. A slightly more detailed presentation of the algorithm is postponed to Sec. 7.7.

Rem. 5.9 means that in case G_σ is a DAG, learning whether $\sigma_{A_1 \ldots A_n}$ is Markov for it already tells us all there is to be found out about the possibilities of any DAG with vertices $A_1, \ldots, A_n$ being a candidate causal explanation. If $\sigma_{A_1 \ldots A_n}$ is Markov for G_σ, the pair forms a faithful QCM. The set of DAGs, which, together with $\sigma_{A_1 \ldots A_n}$, form non-faithful QCMs, are all DAGs with vertices $A_1, \ldots, A_n$, of which G_σ is a subgraph. Generally, the problem of causal inference can be restricted to considering faithful QCMs, since the exact set of non-faithful QCMs is then always trivially known, too, and only given $\sigma_{A_1 \ldots A_n}$, without further clues such as the embedding of the quantum nodes into spacetime, all non-faithful QCMs are indistinguishable. If in turn $\sigma_{A_1 \ldots A_n}$ is not Markov for G_σ, we conclude that there does not exist any DAG with vertices $A_1, \ldots, A_n$ that can causally explain $\sigma_{A_1 \ldots A_n}$.

This sketched naive version of a causal discovery algorithm does not enable one to infer much more, mainly due to the fact that G_σ is generally — that is, in case of non-Markovianity — a little conclusive object, as explained in Sec. 5.7.1. However, in the following special case one can draw an important conclusion from non-Markovianity. Suppose $\sigma_{A_1 \ldots A_n}$ is not Markov, but it is known to be a quantum comb. Then there always exists a unitary process involving further nodes, from which $\sigma_{A_1 \ldots A_n}$ can be seen to arise and which has a DAG as its causal structure and forms a QCM[16]. Thus, given that $\sigma_{A_1 \ldots A_n}$ is a comb, non-Markovianity certifies that there are necessarily latent common causes to at least some of the original nodes $A_1, \ldots, A_n$. This leads to further questions concerning what one can say beyond just that common causes are missing. Can one design an algorithm which is more conclusive and reveals, e.g., which subsets of nodes it is that necessarily need further common causes? Such investigation is left for future work.

Observe the following important difference to classical causal discovery algorithms based on non-interventional data. There, the presence of latent common causes can never be inferred from the given data; it always is a substantial assumption whether there are latent common causes or not — one which has a strong influence on how complex the causal discovery algorithm is [9]. Now, note that there is a completely analogous version of the above causal discovery algorithm for classical processes, just by seeing them as special cases of quantum processes. This

[16]This follows essentially from the results on quantum combs in Ref. [32] by similar arguments as discussed at the end of Sec. 5.2.2. Any quantum comb has a realisation as a quantum network of a similar form as in Fig. 5.4, however, with isometries as the component maps, where Fig. 5.4 shows the unitary maps U_i. Dilating these isometries to unitary maps, a broken unitary circuit is obtained, i.e. a unitary process with a DAG as causal structure, where this step will generally introduce additional common causes.

shows what, if one has access to arbitrary interventions on all variables, the classical problem of causal inference turns into — above all, one notes that it does not trivialise. For instance, one may then similarly infer that there *must be* latent, unobserved common causes.

The conclusion of the presence of latent common causes in case of non-Markovianity is a meaningful one for quantum combs, because there necessarily exists a quantum causal model involving some latent common causes, which constitutes a possible causal explanations of the given process. In contrast, if G_σ is not a DAG, or if it is a DAG, but $\sigma_{A_1 \dots A_n}$ is not a quantum comb, then concluding the need of latent common causes is — at least so far — vacuous, since it is not clear whether $\sigma_{A_1 \dots A_n}$ would have a meaningful causal explanation in any framework. How progress in this direction is possible is what Chap. 7 is dedicated to and Sec. 7.7 will eventually extend the above causal discovery algorithm.

Chapter 6

Causal structure and compositional structure

This chapter presents the results from the second publication in Ref. [2]. The quantum direct-cause relation from Chapter 4 is based on the view that at a fundamental level quantum evolution is unitary and it is in unitary transformations that causal relations reside. As a consequence, every unitary transformation has a causal structure according to Def. 4.3 and so does every unitary process according to Def. 4.7. Chapter 5 presented the framework of quantum causal models based on these definitions. Now, loosely speaking, if Chapter 5 'went up', studying the ramifications from the underlying causal structure at the level of an effective description with generic, non-unitary quantum processes, the direction of inquiry here is to 'go down' and study how a more fine-grained, causal understanding of unitary transformations can be developed. Can the concept of a 'causal mechanism' that mediates the causal influence to a system from its direct causes, be identified more precisely in a compositional manner?

6.1 Introducing the question and prior work

The context, within which to carve out the above vague question a little more concretely in a first step, comes from two lines of research. One tradition is that of studying 'localisability of causal maps' in the sense of, e.g., Refs. [14, 16, 18]. The spirit of these works, which were also mentioned in Chapter 1, can be paraphrased as: given a quantum channel with certain pathways of signalling and assumed spacial relations between the involved systems, studying circuit decompositions such that the channel can be seen to respect a finite speed of signalling since any signalling is mediated through a sequence of 'local interactions' in some circuit. In the first of these works, Ref. [14], Beckmann *et al.* showed in particular that given a bipartite channel with two systems A and B, where A can signal to B, but not vice versa, the channel has a circuit decomposition, where A first interacts with an environment, which then interacts with B[1]. For a tripartite unitary U from ABC to ABC, Schumacher and Westmoreland then showed in Ref. [16] that if A cannot signal to C, then U has a decomposition into a circuit of the form of a bipartite unitary on AB, followed by a unitary on BC. Ref. [18] studies unitary operators U over an arbitrary number of Hilbert spaces and establishes a representation theorem in a similar spirit: given arbitrary no-signalling constraints, it yields a circuit decomposition of U, where systems only interact with their 'nearest neighbours'. There is much further literature in the same vein and with similar results (see, e.g., Refs. [130–133]), and in particular, a large body of literature concerned with the application of such results to 'quantum cellular automata' (see, e.g., [134–143]).

Another tradition emphasises the role of *compositionality* for a better understanding of the quantum formalism. In particular, the category-theoretic approach to quantum theory stands in this tradition and shaped it, above all by leading to the development of a diagrammatical representation of the theory that has become a useful tool for reasoning about quantum systems (see, e.g., Refs. [20, 21, 24, 25] and references therein). Similarly, the framework of 'operational probabilistic theories' emphasises compositional structure and uses a graphical representation thereof (see, e.g., Refs. [19, 26]). As mentioned in Chapter 1, studying causality has played a vital role in all of these, including defining what a 'causal process' is, what makes a theory a 'causal theory', and understanding the link to relativistic causality (see, e.g., Refs. [19, 22, 23, 26, 30]). Nonetheless, a rigorous understanding of the relation between causal structure and compositional structure of unitary transformations is missing – can the former be understood in terms of the latter?

Now, suppose a unitary map U has a representation as a quntum circuit diagram, that is, U is equivalent to the composition of other unitary maps, sequentially and in tensor product. If there is no path from input system A to output system B in the circuit diagram, then there is no influence from A to B in U (see, e.g., Ref. [30]) – the no-influence relation thereby becomes graphically evident in the circuit representation of U. Conversely, the result by Schumacher and Westmoreland from Ref. [16] implies that, given a unitary map U, if A does not influence B, then there always exists a circuit decomposition of U which makes that particular no-influence relation graphically evident through the absence of a corresponding path from A to B.

[1] In their terminology the statement is that a semicausal bipartite channel is semilocalisable.

However, as the next section will argue in detail, not all unitaries allow for a circuit decomposition, which simultaneously makes all no-influence relations evident. Hence, the question of whether causal structure can be understood in compositional terms still stands. The remainder of this chapter will show how progress is possible, essentially, by studying Thm. 4.1 in conjunction with Lem. 4.1 — the recurring main tools to the study of causal structure in this thesis.

6.2 Decompositions using circuit diagrams

This section starts exploring the question whether causal structure of unitary maps can be understood in compositional terms by looking at a few simple examples of unitaries, where corresponding circuit decompositions are known, which achieve a compositional understanding of the respective causal structure. At the same time, these examples will also lead to the limits of circuit decompositions for that purpose.

Consider the simplest case of a unitary map with specified input and output tensor product structures such that the causal structure is nontrivial, i.e. a unitary map with two input and two output subsystems, $U : \mathcal{H}_{A_1} \otimes \mathcal{H}_{A_2} \to \mathcal{H}_{B_1} \otimes \mathcal{H}_{B_2}$. Suppose $A_1 \nrightarrow B_2$ and $A_2 \nrightarrow B_1$. From Thm. 4.1 it follows that $\rho^U_{B_1B_2|A_1A_2} = \rho_{B_1|A_1}\rho_{B_2|A_2}$. Hence, recalling the convention of suppressing identity operators, it holds that $\rho^U_{B_1B_2|A_1A_2} = \rho_{B_1|A_1} \otimes \rho_{B_2|A_2}$. The fact, that $\rho^U_{B_1B_2|A_1A_2}$ represents a unitary channel that factorises into the two channels represented by $\rho_{B_1|A_1}$ and $\rho_{B_2|A_2}$, implies that the latter are unitary channels, too. Therefore, there exist unitary maps $\widetilde{V} : \mathcal{H}_{A_2} \to \mathcal{H}_{B_2}$ and $\widetilde{W} : \mathcal{H}_{A_1} \to \mathcal{H}_{B_1}$, such that $U = \widetilde{W} \otimes \widetilde{V}$ (a result that had been obtained in several previous works; see, e.g., Refs. [14,131,144]). Fig. 6.1 represents this decomposition graphically and makes the two causal constraints, $A_1 \nrightarrow B_2$ and $A_2 \nrightarrow B_1$, graphically evident through the fact that on the right-hand side of it, there is no path from A_1 to B_2 and similarly not from A_2 to B_1.

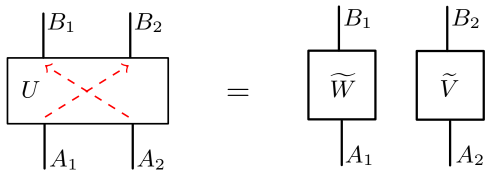


Figure 6.1: Factorisation of unitary U that is implied by $A_1 \nrightarrow B_2 \wedge A_2 \nrightarrow B_1$ (indicated as red dashed arrows).

Next, consider a unitary map with three input and output systems, $U : \mathcal{H}_{A_1} \otimes \mathcal{H}_{A_2} \otimes \mathcal{H}_{A_3} \to \mathcal{H}_{B_1} \otimes \mathcal{H}_{B_2} \otimes \mathcal{H}_{B_3}$. The following result by Schumacher and Westmoreland from Ref. [16] identifies a circuit decomposition of U that is implied by $A_1 \not\twoheadrightarrow B_3$.

Theorem 6.1 [16][2]: *Let* $U : \mathcal{H}_{A_1} \otimes \mathcal{H}_{A_2} \otimes \mathcal{H}_{A_3} \to \mathcal{H}_{B_1} \otimes \mathcal{H}_{B_2} \otimes \mathcal{H}_{B_3}$ *be a unitary. If* $A_1 \not\twoheadrightarrow B_3$*, then there exist unitaries* $V : \mathcal{H}_{A_2} \otimes \mathcal{H}_{A_3} \to \mathcal{H}_X \otimes \mathcal{H}_{B_3}$ *and* $W : \mathcal{H}_{A_1} \otimes \mathcal{H}_X \to \mathcal{H}_{B_1} \otimes \mathcal{H}_{B_2}$ *such that* $U = (W \otimes \mathbb{1}_{B_3})(\mathbb{1}_{A_1} \otimes V)$*.*

Thm. 6.1 is expressed graphically in Fig. 6.2a, where the right-hand side again makes the constraint $A_1 \not\twoheadrightarrow B_3$ evident through the absence of a path from A_1 to B_3. Similarly, in case $A_3 \not\twoheadrightarrow B_1$ holds, a corresponding decomposition as in Fig. 6.2b exists.

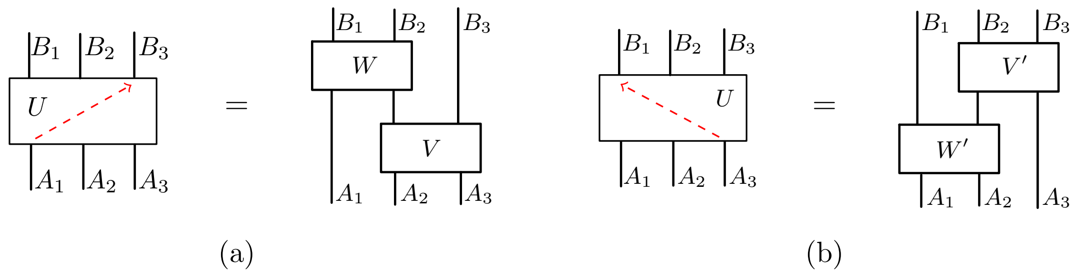


Figure 6.2: Circuit decompositions of unitary U in (a) and (b), which are implied by $A_1 \not\twoheadrightarrow B_3$ and $A_3 \not\twoheadrightarrow B_1$ (indicated as red dashed arrows), respectively.

As the special case of Thm. 6.1 for when the two middle systems (above labelled A_2 and B_2) are trivial systems, observe that if for a 2-input, 2-output unitary map $U : \mathcal{H}_{A_1} \otimes \mathcal{H}_{A_2} \to \mathcal{H}_{B_1} \otimes \mathcal{H}_{B_2}$, it holds that $A_1 \not\twoheadrightarrow B_2$, then there exists a decomposition as in Fig. 6.3a, which makes that causal constraint evident. Similarly, Fig. 6.3b depicts the corresponding decomposition in case $A_2 \not\twoheadrightarrow B_1$ holds.

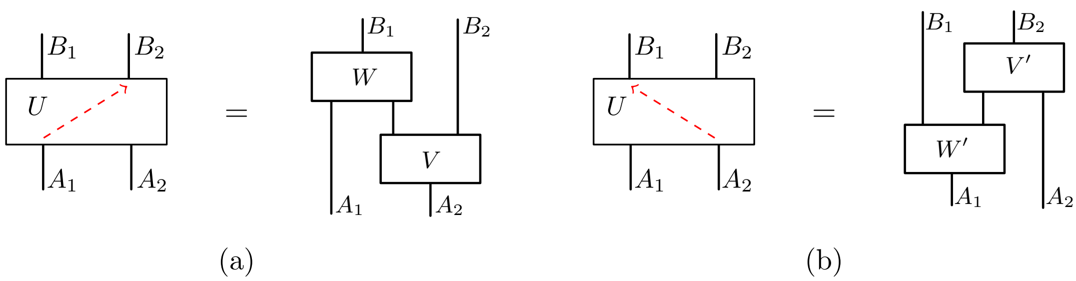


Figure 6.3: Circuit decompositions of unitary U in (a) and (b), which are implied by $A_1 \not\twoheadrightarrow B_2$ and $A_2 \not\twoheadrightarrow B_1$ (indicated as red dashed arrows), respectively.

In case both causal constraints, $A_1 \not\twoheadrightarrow B_2$ and $A_2 \not\twoheadrightarrow B_1$, hold simultaneously for a 2-input, 2-output unitary map, Fig. 6.1 already showed a decomposition that

[2] The result in Ref. [16] is stated for unitaries $U : \mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C \to \mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C$, i.e. for unitaries with the same set of systems as in- and output, but it is straightforward to extend their proof to the more general case stated here.

expresses that fact. Thus, for all presented circuit decompositions of some unitary map U, as long as the assumed causal constraints are the only ones that U satisfies, then the corresponding circuit decomposition faithfully expresses the causal structure of U: there is a path from an input system A to an output system B if and only if there actually is causal influence from A to B.

Now, returning to a 3-input, 3-output unitary map, the obvious question is whether in case $A_1 \nrightarrow B_3$ and $A_3 \nrightarrow B_1$ hold simultaneously, there similarly exists a circuit decomposition that captures the causal structure. Decompositions as in Figs. 6.2a and 6.2b then exist, but neither on their own expresses both constraints. There of course exists a circuit diagram with a corresponding connectivity, namely the one in Fig. 6.4: any unitary map $U : \mathcal{H}_{A_1} \otimes \mathcal{H}_{A_2} \otimes \mathcal{H}_{A_3} \to \mathcal{H}_{B_1} \otimes \mathcal{H}_{B_2} \otimes \mathcal{H}_{B_3}$ defined by a unitary circuit diagram of that form necessarily satisfies $A_1 \nrightarrow B_3$ and $A_3 \nrightarrow B_1$. However, not all unitary maps that satisfy $A_1 \nrightarrow B_3$ and $A_3 \nrightarrow B_1$, admit a circuit decomposition of the form as in Fig. 6.4.

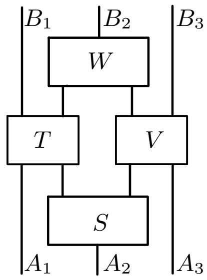


Figure 6.4: Unitary circuit diagram, with the feature that the corresponding unitary transformation satisfies $A_1 \nrightarrow B_3 \wedge A_3 \nrightarrow B_1$.

A simple argument to convince oneself of that fact is the following. Suppose for the unitary $U : \mathcal{H}_{A_1} \otimes \mathcal{H}_{A_2} \otimes \mathcal{H}_{A_3} \to \mathcal{H}_{B_1} \otimes \mathcal{H}_{B_2} \otimes \mathcal{H}_{B_3}$, the conditions $A_1 \nrightarrow B_3$ and $A_3 \nrightarrow B_1$ are the only causal constraints, i.e., in particular A_2 can influence B_1 and also B_3. Furthermore, suppose A_2 is prime-dimensional. If U had a circuit decomposition of the form as in Fig. 6.4, then the intermediate systems between the unitaries S and T as well as S and V, respectively, cannot both be non-trivial systems, because their product is isomorphic to A_2. However, that in turn means that it is impossible for causal influence to go to both, B_1 and B_3. Finally, in order to see that a concrete unitary map with such properties exists, consider $U : \mathcal{H}_{A_1} \otimes \mathcal{H}_{A_2} \otimes \mathcal{H}_{A_3} \to \mathcal{H}_{B_1} \otimes \mathcal{H}_{B_2} \otimes \mathcal{H}_{B_3}$ with all Hilbert spaces two-dimensional and defined as in Fig. 6.5, that is, as a sequential composition of two CNOT gates, both of which have A_2 as the control system, and A_1 and A_3 as the respective target systems (for $i = 1, 2, 3$, B_i is taken to be a copy of A_i here.).

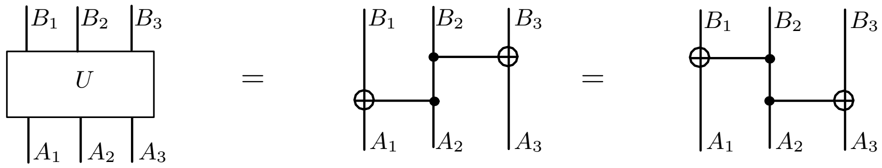


Figure 6.5: Example of a unitary U, satisfying $A_1 \nrightarrow B_3$ and $A_3 \nrightarrow B_1$, which does not have a decomposition of the form of Fig. 6.4.

A first conclusion therefore is that circuit decompositions, i.e. tensor product and sequential compositions of unitary maps, are not in general sufficient to understand causal structure in compositional terms.

6.3 A decomposition beyond circuit diagrams

The open question from above concerning which decomposition of a unitary map $U : \mathcal{H}_{A_1} \otimes \mathcal{H}_{A_2} \otimes \mathcal{H}_{A_3} \to \mathcal{H}_{B_1} \otimes \mathcal{H}_{B_2} \otimes \mathcal{H}_{B_3}$ is implied by the conjunction of the two causal constraints, $A_1 \nrightarrow B_3$ and $A_3 \nrightarrow B_1$, is answered by the following theorem. We will first prove the theorem and then give a graphical representation of the result.

Theorem 6.2 *Given a unitary $U : \mathcal{H}_{A_1} \otimes \mathcal{H}_{A_2} \otimes \mathcal{H}_{A_3} \to \mathcal{H}_{B_1} \otimes \mathcal{H}_{B_2} \otimes \mathcal{H}_{B_3}$, if $A_1 \nrightarrow B_3$ and $A_3 \nrightarrow B_1$, then*

$$U = \Big(\mathbb{1}_{B_1} \otimes T \otimes \mathbb{1}_{B_3}\Big) \ \Big(\bigoplus_{i\in I} V_i \otimes W_i\Big) \ \Big(\mathbb{1}_{A_1} \otimes S \otimes \mathbb{1}_{A_3}\Big) \ , \tag{6.1}$$

where S and T are unitaries, and $\{V_i\}_{i\in I}$ and $\{W_i\}_{i\in I}$ families of unitaries, of the form

$$\begin{aligned} S \ &: \ \mathcal{H}_{A_2} \ \to \ \textstyle\bigoplus_{i\in I} \mathcal{H}_{X_i^L} \otimes \mathcal{H}_{X_i^R} \ , \qquad & V_i \ &: \ \mathcal{H}_{A_1} \otimes \mathcal{H}_{X_i^L} \ \to \ \mathcal{H}_{B_1} \otimes \mathcal{H}_{Y_i^L} \ , \\ T \ &: \ \textstyle\bigoplus_{i\in I} \mathcal{H}_{Y_i^L} \otimes \mathcal{H}_{Y_i^R} \ \to \ \mathcal{H}_{B_2} \ , \qquad & W_i \ &: \ \mathcal{H}_{X_i^R} \otimes \mathcal{H}_{A_3} \ \to \ \mathcal{H}_{Y_i^R} \otimes \mathcal{H}_{B_3} \ . \end{aligned}$$

In order to prove the theorem, the following two lemmas will be essential. The first is a mere restatement of Lem. 4.1 in a more careful way, making explicit the unitary isomorphisms that are implicit in Lem. 4.1 (also see Rem. 4.2).

Lemma 6.1 *Let $\rho_{A|CD}$ and $\rho_{B|DE}$ be CJ representations of channels. If $[\rho_{A|CD} \ , \rho_{B|DE}] = 0$, then there exist a Hilbert space $\mathcal{H}_X = \bigoplus_{i\in I} \mathcal{H}_{X_i^L} \otimes \mathcal{H}_{X_i^R}$, a unitary $S : \mathcal{H}_D \to \mathcal{H}_X$, with transpose $S^T : \mathcal{H}_X^* \to \mathcal{H}_D^*$, and families of channels $\{\rho_{A|CX_i^L}\}_{i\in I}$*

and $\{\rho_{B|X_i^R E}\}_{i\in I}$*, such that*[3]

$$\rho_{A|CD} \;=\; S^T\Big(\bigoplus_{i\in I}\rho_{A|CX_i^L} \;\otimes\; \mathbb{1}_{(X_i^R)^*}\Big)\left(S^T\right)^\dagger \tag{6.2}$$

$$\rho_{B|DE} \;=\; S^T\Big(\bigoplus_{i\in I}\mathbb{1}_{(X_i^L)^*} \;\otimes\; \rho_{B|X_i^R E}\Big)\left(S^T\right)^\dagger \;. \tag{6.3}$$

The channel $\rho_{A|CD}$ *is therefore equivalent to the composition of a channel corresponding to the unitary* $\mathbb{1}_C\otimes S$*, followed by the channel* $\bigoplus_{i\in I}\rho_{A|CX_i^L} \;\otimes\; \mathbb{1}_{(X_i^R)^*}$*. Similarly* $\rho_{B|DE}$*.*

The second lemma relies on the concept of a *reduced unitary channel*, defined in Def. 5.4 in Chap. 5. For ease of reference it is repeated here: A channel $\mathcal{C} : \mathcal{L}(\mathcal{H}_A)\to\mathcal{L}(\mathcal{H}_B)$ is a reduced unitary channel if and only if there exists a unitary transformation $U:\mathcal{H}_A\to\mathcal{H}_B\otimes\mathcal{H}_F$ such that $\rho^{\mathcal{C}}_{B|A} = \mathrm{Tr}_F[\rho^U_{FB|A}]$.

Lemma 6.2 *Let* $\rho_{Y|X}$ *be a reduced unitary channel.*

(1) If X *has a tensor product structure* $\mathcal{H}_X = \mathcal{H}_{X_1}\otimes\mathcal{H}_{X_2}$*, with respect to which* $\rho_{Y|X} = \rho_{Y|X_1}\otimes\mathbb{1}_{X_2}$*, then* $\rho_{Y|X_1}$ *is a reduced unitary channel.*

(2) If $\rho_{Y|X} = \bigoplus_i \rho_{Y|X_i}$ *for some decomposition into orthogonal subspaces* $\mathcal{H}_X = \bigoplus_i \mathcal{H}_{X_i}$*, then* $\rho_{Y|X_i}$ *is a reduced unitary channel for each* i*.*

Proof of Lemma 6.2. See Appendix B.1. □

Proof of Theorem 6.2: Consider a unitary transformation $U:\mathcal{H}_{A_1}\otimes\mathcal{H}_{A_2}\otimes\mathcal{H}_{A_3}\to\mathcal{H}_{B_1}\otimes\mathcal{H}_{B_2}\otimes\mathcal{H}_{B_3}$ such that $A_1\not\rightarrow B_3$ and $A_3\not\rightarrow B_1$. Theorem 4.1 implies that

$$\rho^U_{B_1B_2B_3|A_1A_2A_3} = \rho_{B_1|A_1A_2}\;\rho_{B_2|A_1A_2A_3}\;\rho_{B_3|A_2A_3}\;, \tag{6.4}$$

where all operators commute pairwise. Hence, by Lemma 6.1, there exist a Hilbert space $\mathcal{H}_X = \bigoplus_{i\in I}\mathcal{H}_{X_i^L}\;\otimes\;\mathcal{H}_{X_i^R}$, a unitary $S:\mathcal{H}_{A_2}\to\mathcal{H}_X$, and families of channels $\{\rho_{B_1|A_1X_i^L}\}_{i\in I}$ and $\{\rho_{B_3|X_i^R A_3}\}_{i\in I}$, such that $\rho_{B_1|A_1A_2}$ is equivalent to the composition of the unitary channel corresponding to $\mathbb{1}_{A_1}\otimes S$, followed by $\bigoplus_{i\in I}\rho_{B_1|A_1X_i^L}\otimes\mathbb{1}_{(X_i^R)^*}$, and $\rho_{B_3|A_2A_3}$ is equivalent to the composition of the unitary channel corresponding to $S\otimes\mathbb{1}_{A_3}$, followed by $\bigoplus_{i\in I}\mathbb{1}_{(X_i^L)^*}\;\otimes\;\rho_{B_3|X_i^R A_3}$.

Eq. (6.4) implies that $\rho_{B_1|A_1A_2}\otimes\mathbb{1}_{A_3^*}$ is a reduced unitary channel. Lemma 6.2 then gives that, for each i, $\rho_{B_1|A_1X_i^L}$ is a reduced unitary channel. Similarly, for

[3]The appearance of the transpose of S in this equation is due to our convention of defining Choi-Jamiołkowksi operators as acting on the dual space of the input to the channel.

each i, $\rho_{B_3|X_i^R A_3}$ is a reduced unitary channel. Hence there exist families of unitaries

$$\begin{aligned} V_i &= \mathcal{H}_{A_1} \otimes \mathcal{H}_{X_i^L} \to \mathcal{H}_{B_1} \otimes \mathcal{H}_{Y_i^L} , \\ W_i &= \mathcal{H}_{X_i^R} \otimes \mathcal{H}_{A_3} \to \mathcal{H}_{Y_i^R} \otimes \mathcal{H}_{B_3} \end{aligned}$$

such that $\rho_{B_1|A_1X_i^L} = \mathrm{Tr}_{Y_i^L}[\rho^{V_i}_{B_1Y_i^L|A_1X_i^L}]$ and $\rho_{B_3|X_i^R A_3} = \mathrm{Tr}_{Y_i^R}[\rho^{W_i}_{Y_i^R B_3|X_i^R A_3}]$, where Y_i^L and Y_i^R are some additional output systems of appropriate dimension.

Now consider the unitary transformation

$$\widetilde{U} := \Big(\bigoplus_i V_i \otimes W_i\Big)\Big(\mathbb{1}_{A_1} \otimes S \otimes \mathbb{1}_{A_3}\Big) : \mathcal{H}_{A_1} \otimes \mathcal{H}_{A_2} \otimes \mathcal{H}_{A_3} \to \mathcal{H}_{B_1} \otimes \mathcal{H}_{Y} \otimes \mathcal{H}_{B_3} ,$$

where $\mathcal{H}_Y := \bigoplus_i \mathcal{H}_{Y_i^L} \otimes \mathcal{H}_{Y_i^R}$. By construction, $\rho^{\widetilde{U}}_{B_1YB_3|A_1A_2A_3}$ is a purification of $\rho_{B_1B_3|A_1A_2A_3} = \rho_{B_1|A_1A_2}\rho_{B_3|A_2A_3}$, as is $\rho^{U}_{B_1B_2B_3|A_1A_2A_3}$. By uniqueness of purification up to a unitary transformation on the purifying system, there therefore exists a unitary transformation $T : \mathcal{H}_Y \to \mathcal{H}_{B_2}$ such that

$$U = (\mathbb{1}_{B_1} \otimes T \otimes \mathbb{1}_{B_3})\, \widetilde{U} .$$

This completes the proof. □

The decomposition from Eq. (6.1) can be represented graphically as in Fig. 6.6.

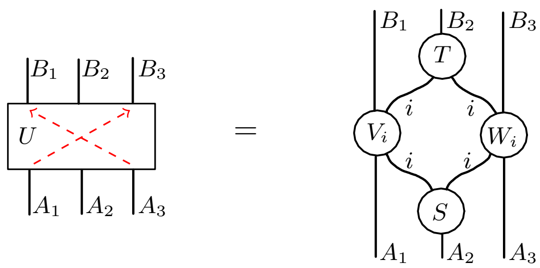


Figure 6.6: Theorem 6.2 written graphically: the decomposition as in Eq. (6.1), implied by $A_1 \not\twoheadrightarrow B_3 \wedge A_3 \not\twoheadrightarrow B_1$, can be represented by an extended circuit diagram as on the right-hand side.

We refer to a diagram as on the right-hand side of Fig. 6.6 as an *extended circuit diagram*. While a general introduction to such diagrams that extend the expressiveness of circuit diagrams, is postponed to the next section, Fig. 6.7 will support the following explanation of how Fig. 6.6 expresses the data from Eq. (6.1).

In a circuit diagram, individual wires represent Hilbert spaces and their parallel composition the corresponding tensor product. Now in Fig. 6.6, wires with an index i on them, such as those between the circles S and V_i and between S and

W_i, respectively, represent the families of Hilbert spaces $\{\mathcal{H}_{X_i^L}\}_i$ and $\{\mathcal{H}_{X_i^R}\}_i$, respectively. These two wires taken together, as parallel wires, represent the space $\bigoplus_{i\in I}\mathcal{H}_{X_i^L}\otimes\mathcal{H}_{X_i^R}$, which is distinct from the space $\left(\bigoplus_{i\in I}\mathcal{H}_{X_i^L}\right)\otimes\left(\bigoplus_{j\in I}\mathcal{H}_{X_j^R}\right)$. The latter contains all cross terms and is what two parallel wires in an ordinary circuit diagram would represent if the individual wires were to represent $\bigoplus_{i\in I}\mathcal{H}_{X_i^L}$ and $\bigoplus_{j\in I}\mathcal{H}_{X_j^R}$, respectively. Similarly, the indexed wires connected to T represent the families $\{\mathcal{H}_{Y_i^L}\}_i$ and $\{\mathcal{H}_{Y_i^R}\}_i$, respectively, and both wires together, as parallel wires, represent the space $\bigoplus_{i\in I}\mathcal{H}_{Y_i^L}\otimes\mathcal{H}_{Y_i^R}$. Concerning the component maps in Fig. 6.6, the circles S and T represent the corresponding unitary maps from Eq. (6.1) and the individual circles labeled V_i and W_i represent the corresponding families of unitaries, while the parallel composition of the circles V_i and W_i represents the unitary map $\bigoplus_{i\in I}V_i\otimes W_i$. Fig. 6.7 also shows three possible slices through the diagram and the respective types of the overall Hilbert space associated with each slice. Reading the diagram bottom up, these are the respective domains and codomains of the three unitaries that are composed sequentially in Eq. (6.1), namely $\mathbb{1}_{A_1}\otimes S\otimes\mathbb{1}_{A_3}$ then $(\bigoplus_{i\in I}V_i\otimes W_i)$ and finally, $\mathbb{1}_{B_1}\otimes T\otimes\mathbb{1}_{B_3}$.

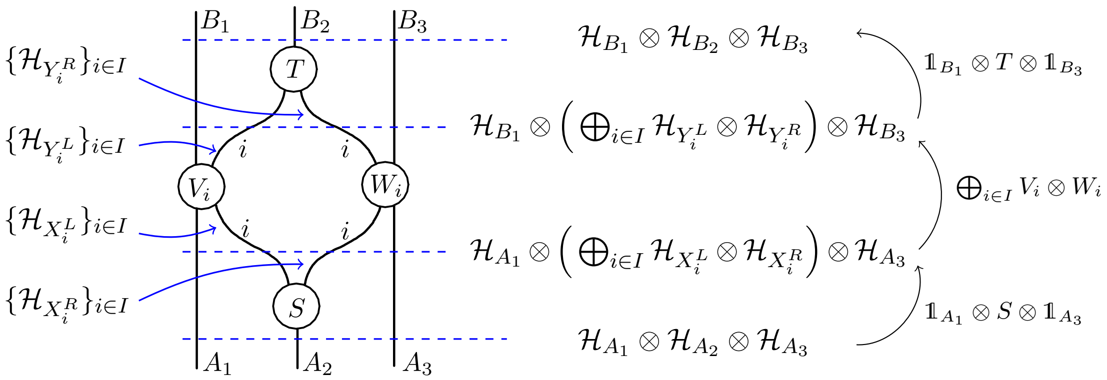


Figure 6.7: Illustration of the data represented by the extended circuit diagram in Fig. 6.6.

In Sec. 6.2 an example of a unitary U was given, defined by the composition of two CNOT gates as in Fig. 6.5, which satisfies $A_1 \nrightarrow B_3$ and $A_3 \nrightarrow B_1$, but cannot be decomposed into a circuit as in Fig. 6.4. It is straightforward to see explicitly what the decomposition of the form as in Fig. 6.6 in this case is. Let $i\in\{0,1\}$ be a binary index, $\mathcal{H}_{X_0^L}$, $\mathcal{H}_{X_0^R}$, $\mathcal{H}_{X_1^L}$ and $\mathcal{H}_{X_1^R}$ one-dimensional Hilbert spaces and $|0\rangle_L\in\mathcal{H}_{X_0^L}$, $|0\rangle_R\in\mathcal{H}_{X_0^R}$, $|1\rangle_L\in\mathcal{H}_{X_1^L}$ and $|1\rangle_R\in\mathcal{H}_{X_1^R}$ some normalised states. The control qubit $\mathcal{H}_{A_2}$ is isomorphic to $\mathcal{H}_X := (\mathcal{H}_{X_0^L}\otimes\mathcal{H}_{X_0^R})\oplus(\mathcal{H}_{X_1^L}\otimes\mathcal{H}_{X_1^R})$ via the unitary S sending $|0\rangle$ to $|0\rangle_L|0\rangle_R$ and $|1\rangle$ to $|1\rangle_L|1\rangle_R$. Let V_0 be the identity on $\mathcal{H}_{A_1}$ and V_1 the NOT gate on $\mathcal{H}_{A_1}$ (suppressing the trivial factors $\mathcal{H}_{X_0^L}$ and $\mathcal{H}_{X_1^L}$ in the domain and codomain of V_0 and V_1) and similarly for W_0 and W_1 on $\mathcal{H}_{A_3}$. Finally, letting $T = S^\dagger$, the composition of these unitary maps as in Fig. 6.6 indeed gives U as defined in Fig. 6.5.

Just as the circuit decompositions from Sec. 6.2, Fig. 6.6 has the desired property that if $A_1 \nrightarrow B_3$ and $A_3 \nrightarrow B_1$ are the only causal constraints, then it makes the *causal structure* of U evident through the presence of paths between input and output spaces whenever there is corresponding causal influence.

Note that a unitary map $U : \mathcal{H}_{A_1} \otimes \mathcal{H}_{A_2} \otimes \mathcal{H}_{A_3} \to \mathcal{H}_{B_1} \otimes \mathcal{H}_{B_2} \otimes \mathcal{H}_{B_3}$ that satisfies $A_1 \nrightarrow B_3$ and $A_3 \nrightarrow B_1$ is particularly pertinent to the quantum causal model approach, seeing as it is exactly the kind of unitary transformation that is asserted to exist if A_2 is the *complete common cause* of B_1 and B_3 [4][4] (see Def. 3.10). Thm. 6.2 thus allows one to understand how in general the causal influence from the complete common cause A_2 goes to B_1 and B_3 — it does so 'within subspaces'.

6.4 Extending circuit diagrams

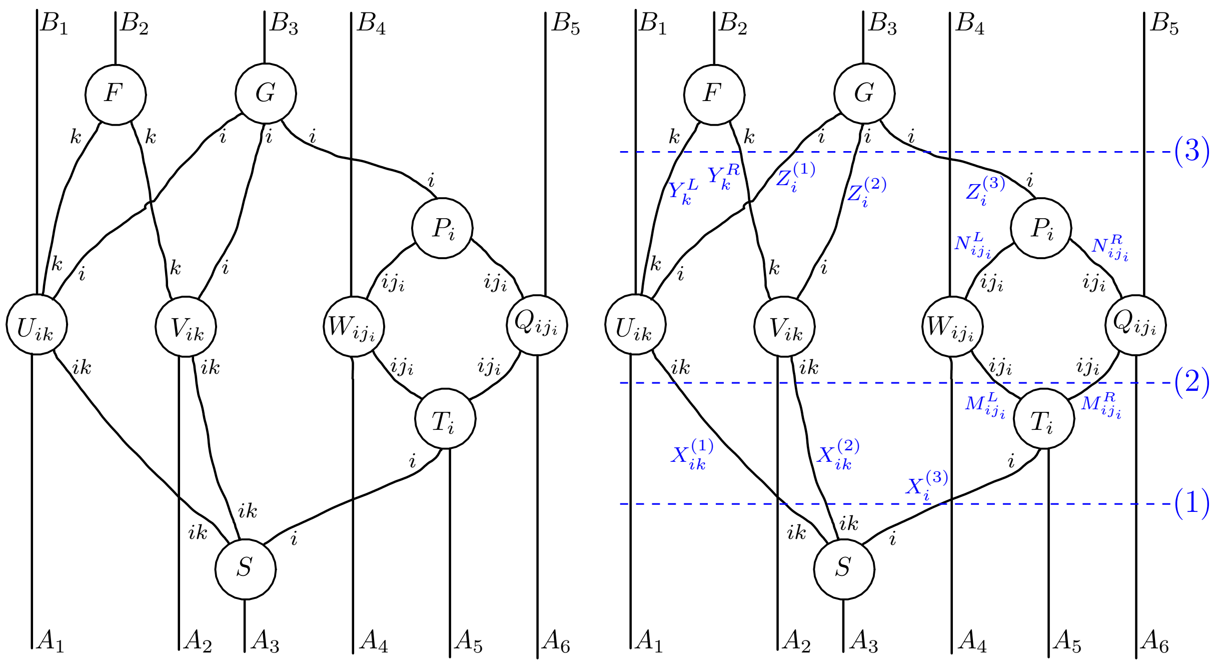
The above proof of Thm. 6.2 and the graphical representation of that result in Fig. 6.6 are exemplary of both main aspects of this chapter: the development of proof techniques for deriving decompositions of unitary transformations that are implied by their particular causal structures, and the development of a graphical representation of those compositional structures, namely *extended circuit diagrams*. In this thesis the focus lies on the former, while the rigorous presentation of a graphical language with syntax and semantics that formalises the extended circuit diagrams is left for future work. The present section will therefore content itself with the informal explanation of the example of a generic extended circuit diagram in Fig 6.8a, which contains all basic features needed to state the results in Sec. 6.6.

The following will step by step explain what data is represented by the different kinds of wires and circles and, eventually, by the entire diagram.

What do the wires represent?

A plain wire represents a Hilbert space, just as in circuit diagrams. A wire with an index, or in general a tuple of indices, next to it is associated with a family of Hilbert spaces, parametrised by that tuple of indices. It is the convention that the set, in which an index i takes values, has the corresponding capital letter, i.e. $i \in I$.

[4] In Ref. [4] a circle-shaped structure, reminiscent of the role S plays in Fig. 6.6, was used for the first time to represent a space of the structure $\bigoplus_{i\in I} \mathcal{H}_{X_i^L} \otimes \mathcal{H}_{X_i^R}$, in order to express the specific block-diagonal structure of the marginal channel $\rho_{B_1B_3|A_1A_2A_3}$.



(a) (b)

Figure 6.8: Example of an extended circuit diagram in (a) and in (b) the same diagram with (in blue) three example slices and explicit labels for the intermediate wires.

The label for the family of Hilbert spaces is typically suppressed in the diagram, only leaving the index behind to indicate the fact that it is a family. Fig. 6.8b has explicit labels of the Hilbert spaces in blue for the purpose of this exposition. For instance, the wire going from the circle S to the circle U_{ik} carries the tuple (i, k) and represents the family of Hilbert spaces $\{\mathcal{H}_{X^{(1)}_{ik}}\}_{i\in I, k\in K}$. Note that in a tuple of indices like (i, j_i), parametrising a family of Hilbert spaces $\{\mathcal{H}_{M^L_{ij_i}}\}_{i\in I, j_i\in J_i}$, we allow an index $j_i \in J_i$ to take values in a set which itself is parametrised by $i \in I$ and refer to this as 'nesting of indices'.

This thesis focuses on extended circuit diagrams, where open in- or outgoing wires do not carry indices. Reading extended circuit diagrams bottom up, indices 'go in loops', introduced by a 'source' circle, such as S for the indices i and k, and disappear in a 'sink' circle, such as F for the index k.

What type is associated with a slice through the diagram?

The overall Hilbert space associated with a slice through the diagram, can be described as follows. Consider the Cartesian product $I \times J \times M \times ...$ of all distinct index sets appearing across the slice, i.e. M appears only once even if the index m

appears on several crossed wires. For each fixed tuple of indices $(i, j, m, ...)$ consider for each crossed wire the corresponding element of its family of Hilbert spaces and form their tensor product. Finally, the overall Hilbert space associated with the slice is obtained from forming the direct sum over these tensor products, summing over all appearing indices[5].

The example slices in Fig. 6.8b are associated with the following Hilbert spaces:

$$(1): \ \mathcal{H}_{A_1} \otimes \mathcal{H}_{A_2} \otimes \Big[\bigoplus_{i\in I, k\in K} \mathcal{H}_{X^{(1)}_{ik}} \otimes \mathcal{H}_{X^{(2)}_{ik}} \otimes \mathcal{H}_{X^{(3)}_{i}} \Big] \otimes \mathcal{H}_{A_4} \otimes \mathcal{H}_{A_5} \otimes \mathcal{H}_{A_6},$$

$$(2): \ \mathcal{H}_{A_1} \otimes \Big[\bigoplus_{i\in I, k\in K} \mathcal{H}_{X^{(1)}_{ik}} \otimes \mathcal{H}_{A_2} \otimes \mathcal{H}_{X^{(2)}_{ik}} \otimes \mathcal{H}_{A_4} \otimes \Big(\bigoplus_{j_i\in J_i} \mathcal{H}_{M^L_{ij_i}} \otimes \mathcal{H}_{M^R_{ij_i}} \Big) \Big] \otimes \mathcal{H}_{A_6},$$

$$(3): \ \mathcal{H}_{B_1} \otimes \Big(\bigoplus_{k\in K} \mathcal{H}_{Y^L_k} \otimes \mathcal{H}_{Y^R_k} \Big) \otimes \Big(\bigoplus_{i\in I} \mathcal{H}_{Z^{(1)}_i} \otimes \mathcal{H}_{Z^{(2)}_i} \otimes \mathcal{H}_{Z^{(3)}_i} \Big) \otimes \mathcal{H}_{B_4} \otimes \mathcal{H}_{B_5} \ .$$

From now on, where there is no ambiguity, we omit the index set I in '$\bigoplus_i$'.

What do the circles represent?

A circle with label S represents a unitary map S with its domain (codomain) given by the Hilbert space associated with the slice through the ingoing (outgoing) wires of S in the sense as described above, i.e. the indices appearing on those wires are summed over in the 'orchestrated' way that respects which wires share the same indices. A circle with an indexed label T_i represents an accordingly parametrised family of unitary maps $\{T_i\}_{i\in I}$, where each T_i is a unitary map with the domain (codomain) Hilbert space similarly determined by the ingoing (outgoing) wires with all indices summed over apart from i, i.e. it is the ith subspace of the Hilbert space associated with the slice through its ingoing (outgoing) wires.

The component unitaries appearing in Fig 6.8a are of the following form:

$$F : \bigoplus_k \mathcal{H}_{Y^L_k} \otimes \mathcal{H}_{Y^R_k} \to \mathcal{H}_{B_2} \ , \qquad U_{ik} : \mathcal{H}_{A_1} \otimes \mathcal{H}_{X^{(1)}_{ik}} \to \mathcal{H}_{B_1} \otimes \mathcal{H}_{Y^L_k} \otimes \mathcal{H}_{Z^{(1)}_i} \ ,$$

$$G : \bigoplus_i \mathcal{H}_{Z^{(1)}_i} \otimes \mathcal{H}_{Z^{(2)}_i} \otimes \mathcal{H}_{Z^{(3)}_i} \to \mathcal{H}_{B_3} \ , \qquad V_{ik} : \mathcal{H}_{A_2} \otimes \mathcal{H}_{X^{(2)}_{ik}} \to \mathcal{H}_{Y^R_k} \otimes \mathcal{H}_{Z^{(2)}_i} \ ,$$

$$P_i : \bigoplus_{j_i} \mathcal{H}_{N^L_{ij_i}} \otimes \mathcal{H}_{N^R_{ij_i}} \to \mathcal{H}_{Z^{(3)}_i} \ , \qquad W_{ij_i} : \mathcal{H}_{A_4} \otimes \mathcal{H}_{M^L_{ij_i}} \to \mathcal{H}_{B_4} \otimes \mathcal{H}_{N^L_{ij_i}} \ ,$$

$$T_i : \mathcal{H}_{X^{(3)}_i} \otimes \mathcal{H}_{A_5} \to \bigoplus_{j_i} \mathcal{H}_{M^L_{ij_i}} \otimes \mathcal{H}_{M^R_{ij_i}} \ , \qquad Q_{ij_i} : \mathcal{H}_{M^R_{ij_i}} \otimes \mathcal{H}_{A_6} \to \mathcal{H}_{N^R_{ij_i}} \otimes \mathcal{H}_{B_5} \ ,$$

$$S : \mathcal{H}_{A_3} \to \bigoplus_{i,k} \mathcal{H}_{X^{(1)}_{ik}} \otimes \mathcal{H}_{X^{(2)}_{ik}} \otimes \mathcal{H}_{X^{(3)}_{i}} \ .$$

[5]The type is taken to be fixed up to some distributivity isomorphism (with respect to $\otimes$ and $\oplus$).

Which overall unitary is represented by the diagram?

The unitary represented by an extended circuit diagram is obtained from: (1) composing the component unitaries sequentially and in tensor product according to the connectivity of the diagram as if it was an ordinary circuit diagram, that is, as if ignoring the direct sum structure indicated by the indices, and then (2) adding direct sum symbols with a summation over all indices that appear in the subscripts of the circles' labels, such that the direct sum applies to all terms carrying the respective index.

For instance, the unitary represented by the extended circuit diagram in Fig. 6.8a, expressed in terms of the component unitaries, is the following:

$$\begin{aligned} U \;=\;& \Big(\mathbb{1}_{B_1} \otimes F \otimes G \otimes \mathbb{1}_{B_4 B_5}\Big) \\ & \Bigg[\bigoplus_{i,k} U_{ik} \otimes V_{ik} \otimes \Big[\Big(\mathbb{1}_{B_4} \otimes P_i \otimes \mathbb{1}_{B_5}\Big) \Big(\bigoplus_{j_i} W_{ij_i} \otimes Q_{ij_i}\Big) \Big(\mathbb{1}_{A_4} \otimes T_i \otimes \mathbb{1}_{A_6}\Big) \Big] \Bigg] \\ & \Big(\mathbb{1}_{A_1 A_2} \otimes S \otimes \mathbb{1}_{A_4 A_5 A_6}\Big) \;, \end{aligned}$$

where the 'distributivity isomorphisms' for well-typed composition are suppressed, just as we did in Eq. (6.4) and as will be done henceforth.

A diagram without any indices on its wires is just an ordinary circuit diagram, but for the sake of consistent style they will at times be drawn with 'circles' rather than 'boxes'.

6.5 Causal faithfulness and the hypothesis

The main conclusion from Sec. 6.2 was that circuit decompositions of unitary transformations generally do not allow to understand their causal structure, since in general no single circuit decomposition can express *all* causal constraints. The main insight from Thm. 6.2 then was that, in addition to tensor product and sequential composition, also direct sum structures are necessary for such understanding. This led to the introduction of extended circuit diagrams to represent compositions of unitary maps in the enlarged set of operations. The obvious question now is whether this is sufficient, that is, whether any unitary transformation has a decomposition that allows to understand its causal structure and is expressible as an extended circuit diagram.

In order to formulate a precise hypothesis that this is the case, call an extended circuit diagram that represents a unitary transformation U, *causally faithful* if it holds that there is a path from input system A to output system B in the diagram if and only if there is causal influence from A to B through U[6].

Hypothesis 1 *Every finite-dimensional unitary transformation with specified tensor product structures of n input and k output subsystems, $U : \mathcal{H}_{A_1} \otimes ... \otimes \mathcal{H}_{A_n} \to \mathcal{H}_{B_1} \otimes ... \otimes \mathcal{H}_{B_k}$, can be represented with a causally faithful extended circuit diagram.*

If the unitary map U is represented by a (faithful) extended circuit diagram, then also the represented decomposition of U, seen algebraically, will be called a (faithful) extended circuit decomposition. Two final pieces of notation will be useful to help classify unitary maps and their causal structures. First, a unitary transformation with n input systems and k output systems will be referred to as a *unitary of type* (n, k). Second, given a unitary map $U : \mathcal{H}_{A_1} \otimes ... \otimes \mathcal{H}_{A_n} \to \mathcal{H}_{B_1} \otimes ... \otimes \mathcal{H}_{B_k}$, its causal structure is conveniently represented graphically as a *hypergraph* with vertices given by the set of input systems $A_1, \ldots, A_n$ and k hyperedges defined by the parental sets $\{Pa(B_i)\}_{i=1}^{k}$. See Fig. 6.9 for an example. For better visibility distinct hyperedges will be drawn with distinct colours. Where it matters which hyperedge represents which output system's causal parents, the corresponding association of the latter with colours will be given, otherwise, like in Fig. 6.9, this is left implicit seeing as the advantage of this notation is to make the overlap structure between causal parents evident and differences in possible causal structure arising from a permutation of the output systems often is not of interest.

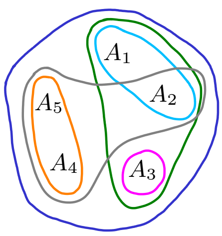


Figure 6.9: Example of the causal structure of a unitary of type $(5, 6)$, represented as a hypergraph with 5 vertices $A_1, ..., A_5$, and 6 hyperedges given by the 6 parental sets $\{A_3\}$, $\{A_1, A_2\}$, $\{A_1, A_2, A_3\}$, $\{A_4, A_5\}$, $\{A_2, A_4, A_5\}$, and $\{A_1, A_2, A_3, A_4, A_5\}$.

6.6 Decompositions of unitary transformations

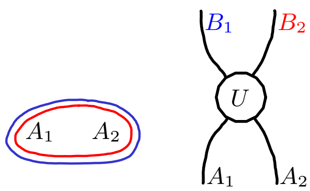
While Hypothesis 1 remains unproven, we do not know of any counter example and the following will present results on causally faithful extended circuit decompositions

[6]This is distinct from the notion of faithfulness of a quantum causal model, although related in spirit in so far as they both obtain whenever either all paths in an extended circuit diagram or all arrows in the DAG of a quantum causal model have the expected meaning.

for unitary maps of type (n, k) with increasing values of n and k, starting with $(2, 2)$.

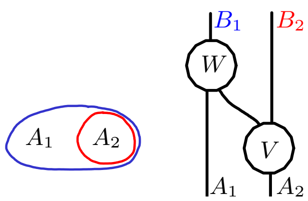
6.6.1 Unitaries of type $(2, 2)$

Any unitary transformation U of type $(2, 2)$ has, up to relabeling, one of the following causal structures in Fig. 6.10a, 6.11a or 6.12a. In the first case, the representation of U in Fig. 6.10b is already a causally faithful circuit diagram. It is generally the case that for any type (n, k), if there are no causal constraints, i.e. all k output systems are influenced by all n input systems, then there is no decomposition that would be informative in causal terms. This case will henceforth be ignored for larger values of n and k. That the causal structures in Figs. 6.11a and 6.12a imply causally faithful circuit decompositions as in Fig. 6.11b and Fig. 6.12b, respectively, was already observed in Sec. 6.2.



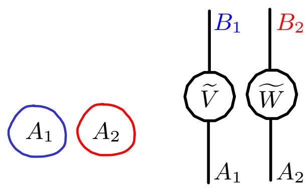
(a) (b)

Figure 6.10



(a) (b)

Figure 6.11



(a) (b)

Figure 6.12

6.6.2 Unitaries of type $(n, 2)$ and $(2, k)$ for $n, k \geq 3$

Before analysing $(n, 2)$ cases, it is useful to first establish a general observation.

Theorem 6.3 *Let $U : \mathcal{H}_{A_1} \otimes ... \otimes \mathcal{H}_{A_n} \to \mathcal{H}_{B_1} \otimes ... \otimes \mathcal{H}_{B_k}$ be a unitary. For any bi-partition of the k output systems into S and $\overline{S} = \{B_1, ..., B_k\} \setminus S$, and any partitioning of the inputs $\{A_1, ..., A_n\}$ into disjoint subsets $P_S \cup C \cup P_{\overline{S}}$, such that $P_S \not\twoheadrightarrow \overline{S}$ and $P_{\overline{S}} \not\twoheadrightarrow S$, there exist Hilbert spaces $\mathcal{H}_{X^L}$ and $\mathcal{H}_{X^R}$ and unitaries $T : \mathcal{H}_C \to \mathcal{H}_{X^L} \otimes \mathcal{H}_{X^R}$, $V : \mathcal{H}_{P_S} \otimes \mathcal{H}_{X^L} \to \mathcal{H}_S$ and $W : \mathcal{H}_{X^R} \otimes \mathcal{H}_{P_{\overline{S}}} \to \mathcal{H}_{\overline{S}}$ such that $U = (V \otimes W)\ (\mathbb{1}_{P_S} \otimes T \otimes \mathbb{1}_{P_{\overline{S}}})$.*

Proof: Seeing as $Pa(S) \subseteq P_S \cup C$ and $Pa(\overline{S}) \subseteq C \cup P_{\overline{S}}$, Theorem 4.1 implies that $\rho^U_{S\overline{S}|P_S C P_{\overline{S}}} = \rho_{S|P_S C}\ \rho_{\overline{S}|C P_{\overline{S}}}$. Lemma 6.1 then implies that there exist a unitary $T : \mathcal{H}_C \to \bigoplus_i \mathcal{H}_{X_i^L} \otimes \mathcal{H}_{X_i^R}$, and families of channels $\{\rho_{S|P_S X_i^L}\}_i$ and $\{\rho_{\overline{S}|X_i^R P_{\overline{S}}}\}_i$, such that $\rho^U_{S\overline{S}|P_S C P_{\overline{S}}} = T^T \Big(\bigoplus_i \rho_{S|P_S X_i^L} \otimes \rho_{\overline{S}|X_i^R P_{\overline{S}}} \Big) \left(T^T\right)^\dagger$. The fact that $\rho^U_{S\overline{S}|P_S C P_{\overline{S}}}$ is a rank 1 operator implies that there cannot be more than one term in the direct sum. Hence, we can write $\mathcal{H}_X = \mathcal{H}_{X^L} \otimes \mathcal{H}_{X^R}$, such that $\rho^U_{S\overline{S}|P_S C P_{\overline{S}}} = T^T \Big(\rho_{S|P_S X^L} \otimes$

$\rho_{\overline{S}|X^R P_{\overline{S}}}\Big) \left(T^T\right)^\dagger$. The operator $\rho_{S|P_S X^L} \otimes \rho_{\overline{S}|X^R P_{\overline{S}}}$ represents a unitary channel, hence each of $\rho_{S|P_S X^L}$ and $\rho_{\overline{S}|X^R P_{\overline{S}}}$ represent unitary channels. Denoting the associated unitaries V and W, respectively, concludes the proof. $\square$

The statement of Thm. 6.3 is expressed graphically in Fig. 6.13.

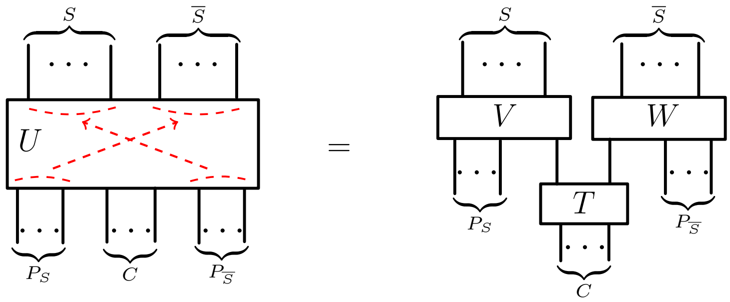


Figure 6.13: Theorem 6.3 written graphically: if U satisfies $P_S \not\rightarrow \overline{S}$ and $P_{\overline{S}} \not\rightarrow S$, then it has a circuit decomposition as on the right-hand side.

Remark 6.1 *It is straightforward to verify that the causal structure of the component unitaries V and W are as expected: if $B_i \in S$ and $Pa^U(B_i) \cap C = \emptyset$ then $Pa^V(B_i) = Pa^U(B_i)$, and otherwise $Pa^V(B_i) = (Pa^U(B_i) \setminus C) \cup \{X^L\}$. Analogously for W if $B_i \in \overline{S}$.*

Note that for a unitary $U : \mathcal{H}_{A_1} \otimes \mathcal{H}_{A_2} \otimes \mathcal{H}_{A_3} \to \mathcal{H}_{B_1} \otimes \mathcal{H}_{B_2} \otimes \mathcal{H}_{B_3}$ that satisfies $A_1 \not\rightarrow B_3$, Thm. 6.3 recovers Thm. 6.1 from Ref. [16] for the choices $S = \{B_1, B_2\}$, $P_S = \{A_1\}$, $C = \{A_2, A_3\}$, $\overline{S} = \{B_3\}$ and $P_{\overline{S}} = \emptyset$.

A decomposition as it is asserted to exist by Thm. 6.3 makes the constraints $P_S \not\rightarrow \overline{S}$ and $P_{\overline{S}} \not\rightarrow S$ evident, but is in general not a causally faithful decomposition. However, in case of a unitary transformation of type $(n, 2)$ for $n \geq 3$, it automatically yields a causally faithful one. Given a unitary $U : \mathcal{H}_{A_1} \otimes ... \otimes \mathcal{H}_{A_n} \to \mathcal{H}_{B_1} \otimes \mathcal{H}_{B_2}$, let $S := \{B_1\}$, $\overline{S} := \{B_2\}$, $P_{12} := Pa(B_1) \cap Pa(B_2)$, $P_1 := Pa(B_1) \setminus P_{12}$ and $P_2 := Pa(B_2) \setminus P_{12}$. Noting that some of the sets P_1, P_{12} or P_2 may be empty, the causal structure of U can be seen to always be of the form as in Fig. 6.14a. Thm. 6.3 then yields a causally faithful circuit decomposition of U as shown in Fig. 6.14b. The special case of $P_{12} = \emptyset$ generalises the situation in Fig. 6.12 and the case $P_2 = \emptyset$ the one in Fig. 6.11.

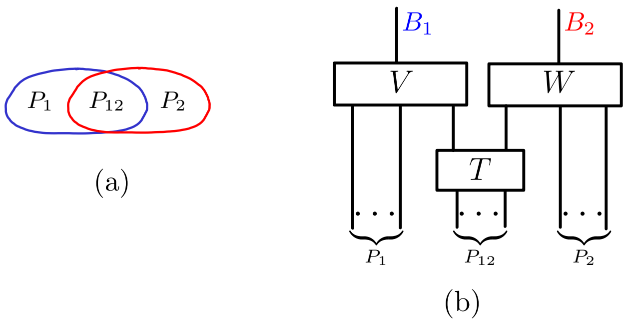


Figure 6.14: The causal structure of a type $(n, 2)$ unitary U can always be cast as in (a), where $P_{12} := Pa(B_1) \cap Pa(B_2)$, $P_1 := Pa(B_1) \setminus P_{12}$ and $P_2 := Pa(B_2) \setminus P_{12}$. Then U has a causally faithful circuit decomposition as in (b).

The following theorem will be instructive for the analysis of the $(2, k)$ cases and, in fact, for arbitrary (n, k) cases, as well as it is an interesting fact in its own right: it establishes a 'reversibility' of the causal structure of unitary transformations [7] (also see discussion in Sec. 8.3).

Theorem 6.4 *If $U : \mathcal{H}_{A_1} \otimes ... \otimes \mathcal{H}_{A_n} \to \mathcal{H}_{B_1} \otimes ... \otimes \mathcal{H}_{B_k}$ is a unitary transformation with causal structure $\{Pa^U(B_j)\}_{j=1}^k$, then the causal structure of $U^\dagger$ is obtained by inverting all causal arrows. That is,*

$$Pa^{U^\dagger}(A_i) \;=\; Ch^U(A_i) \;\; \forall\, i = 1, ..., n \;, \tag{6.5}$$

where $Pa^{U^\dagger}(A_i)$ denotes the parents of A_i in $U^\dagger$, and $Ch^U(A_i)$ denotes the children of A_i in U.

Proof: See App. B.2. □

[7] There is a similar result in Ref. [18]. Whenever U is a unitary operator, i.e. if the factorizations into subsystems for the input and the output Hilbert space are identical, then Thm. 6.4 can be obtained from the result in Ref. [18] (Proposition 2 therein), by observing that the causal structure of such U induces a 'quantum labeled graph', relative to which U is causal in the sense as defined in Ref. [18].

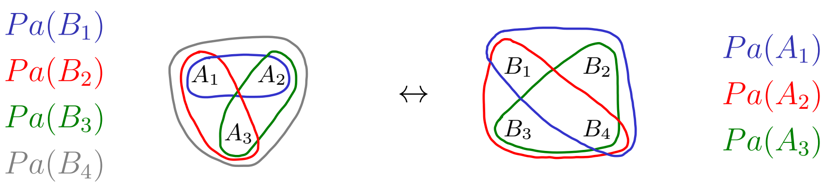


Figure 6.15: Example to illustrate Theorem 6.4 using the hypergraph notation. The two causal structures of a unitary of type $(3, 4)$ on the left-hand side and of a unitary of type $(4, 3)$ on the right-hand side are 'dual' to each other.

Given Thm. 6.4, the following is an immediate consequence.

Proposition 6.1 *Given an extended circuit diagram $\mathcal{C}$, let $\mathcal{C}^\dagger$ be the extended circuit diagram obtained by reading $\mathcal{C}$ from top to bottom, and replacing all unitary transformations featuring in $\mathcal{C}$ with their inverses. If $\mathcal{C}$ represents a type (n, k) unitary U, then $\mathcal{C}^\dagger$ represents the type (k, n) unitary $U^\dagger$. If $\mathcal{C}$ is causally faithful for U, then $\mathcal{C}^\dagger$ is causally faithful for $U^\dagger$.*

The number of distinct causal structures for which independent causally faithful extended circuit decompositions have to be derived is thereby reduced considerably — the reason it is not quite halved is that some causal structures of type (n, n) are symmetric under taking the inverse of the unitary map, i.e. for some unitary maps of type (n, n) the parental sets and the children sets have the same overlap structure amongst themselves.

In particular, given a type $(2, k)$ unitary $U : \mathcal{H}_{A_1} \otimes \mathcal{H}_{A_2} \to \mathcal{H}_{B_1} \otimes ... \otimes \mathcal{H}_{B_k}$, let $C_{12} := Ch(A_1) \cap Ch(A_2)$, $C_1 := Ch(A_1) \setminus C_{12}$ and $C_2 := Ch(A_2) \setminus C_{12}$. Due to Prop. 6.1 and the causally faithful circuit decomposition from Fig. 6.14b for any type $(k, 2)$ unitary, it follows that U has a causally faithful circuit decomposition as in Fig. 6.16.

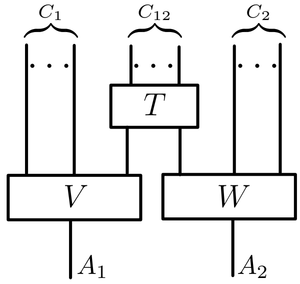
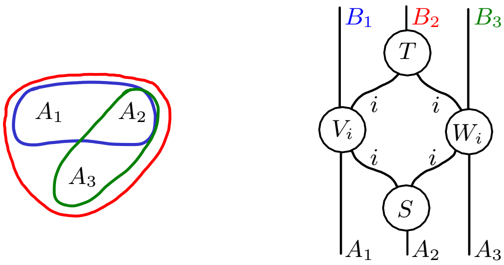


Figure 6.16: Every unitary of type $(2, k)$ has a causally faithful circuit diagram of the above form, where $C_{12} := Ch(A_1) \cap Ch(A_2)$, $C_1 := Ch(A_1) \setminus C_{12}$ and $C_2 := Ch(A_2) \setminus C_{12}$.

6.6.3 Unitaries of type $(3,3)$

This subsection will show that all unitary transformations of type $(3,3)$ have causally faithful (extended) circuit decompositions. One prominent $(3,3)$ case was already covered by Thm. 6.2 and discussed in detail in Sec. 6.3: given a unitary $U : \mathcal{H}_{A_1} \otimes \mathcal{H}_{A_2} \otimes \mathcal{H}_{A_3} \to \mathcal{H}_{B_1} \otimes \mathcal{H}_{B_2} \otimes \mathcal{H}_{B_3}$, if the causal structure of U is as in Fig. 6.17a, then U has a causally faithful extended circuit decomposition as in Fig. 6.17b.

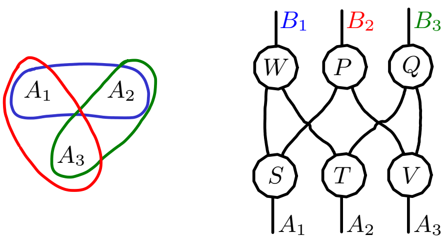


(a) (b)

Figure 6.17

As it turns out, this is the only case that requires an extended circuit diagram, and all other causal structures of type $(3,3)$ unitaries imply the existence of a causally faithful circuit decomposition. Among those there is only one further case, where the proof is not entirely obvious.

Theorem 6.5 *Given a unitary transformation* $U : \mathcal{H}_{A_1} \otimes \mathcal{H}_{A_2} \otimes \mathcal{H}_{A_3} \to \mathcal{H}_{B_1} \otimes \mathcal{H}_{B_2} \otimes \mathcal{H}_{B_3}$*, if the causal structure of* U *is as in Fig. 6.18a, then* U *has a causally faithful circuit diagram as in Fig. 6.18b.*



(a) (b)

Figure 6.18

Proof: See App. B.3. □

The following set of rules will be useful for the remaining $(3,3)$ cases, as well as for many other cases later. We say a (n,k) case *reduces to* a (n',k') case with

$n' \leq n, k' \leq k$ if it holds that in case a causally faithful extended circuit decomposition for the (n', k') case is known, then also one for the (n, k) case is known.

Rules of reduction: Let $U : \mathcal{H}_{A_1} \otimes ... \otimes \mathcal{H}_{A_n} \to \mathcal{H}_{B_1} \otimes ... \otimes \mathcal{H}_{B_k}$ be a unitary transformation of type (n, k) with causal structure $\{Pa(B_j)\}_{j=1}^{k}$.

(R1) *If there is a single-parent output, the problem reduces to a $(n, k-1)$ case:* Suppose $|Pa(B_j)| = 1$ for some $j \in \{1, ..., k\}$. Assume $Pa(B_j) = \{A_i\}$ and write $\overline{A_i} := \{A_1, ..., A_n\} \setminus \{A_i\}$ and $\overline{B_j} := \{B_1, ..., B_k\} \setminus \{B_j\}$. Then $U = (\mathbb{1}_{B_j} \otimes W)(T \otimes \mathbb{1}_{\overline{A_i}})$ for some unitaries $T : \mathcal{H}_{A_i} \to \mathcal{H}_{B_j} \otimes \mathcal{H}_X$ and $W : \mathcal{H}_X \otimes \mathcal{H}_{\overline{A_i}} \to \mathcal{H}_{\overline{B_j}}$, where W is a unitary of type $(n, k-1)$ with causal structure identical to that of U, ignoring $Pa(B_j)$ and replacing A_i with X in all other parental sets. See Fig. 6.19.

(R2) *If there is a single-child input, the problem reduces to a $(n-1, k)$ case:* Suppose $|Ch(A_i)| = 1$ for some $i \in \{1, ..., n\}$. Assume $Ch(A_i) = \{B_j\}$ and write $\overline{A_i} := \{A_1, ..., A_n\} \setminus \{A_i\}$ and $\overline{B_j} := \{B_1, ..., B_k\} \setminus \{B_j\}$. Then $U = (T \otimes \mathbb{1}_{\overline{B_j}})(\mathbb{1}_{A_i} \otimes W)$, for some unitaries $W : \mathcal{H}_{\overline{A_i}} \to \mathcal{H}_X \otimes \mathcal{H}_{\overline{B_j}}$ and $T : \mathcal{H}_{A_i} \otimes \mathcal{H}_X \to \mathcal{H}_{B_j}$, where W is a unitary of type $(n-1, k)$ with the causal structure $Pa^W(B_l) = Pa^U(B_l)$ for all $l \neq j$ and $Pa^W(X) = Pa^U(B_j) \setminus \{A_i\}$. See Fig. 6.20.

(R3) *If there are two identical parental sets, the problem reduces to a $(n, k-1)$ case:* Suppose $Pa(B_j) = Pa(B_{j'})$ for some $j \neq j'$. Considering the two output systems as a composite system, $\mathcal{H}_{\widetilde{B}} := \mathcal{H}_{B_j} \otimes \mathcal{H}_{B_{j'}}$, defines a unitary of type $(n, k-1)$. Any causally faithful extended circuit diagram for the latter obviously induces one for the original case.

(R4) *If there are two identical children sets, the problem reduces to a $(n-1, k)$ case:* Analogous to (R3).

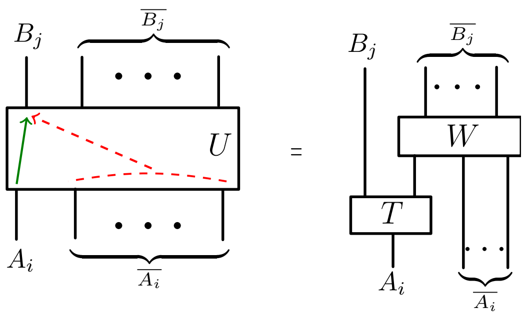


Figure 6.19: Illustration of (R1).

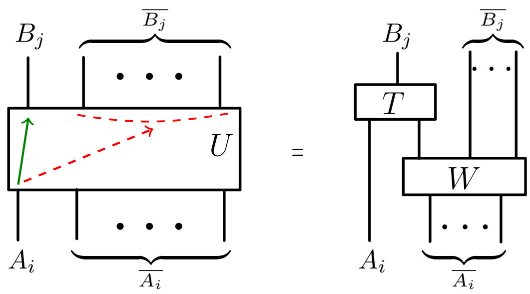
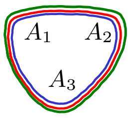
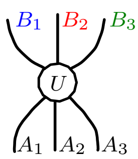
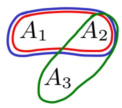
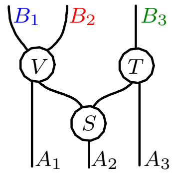
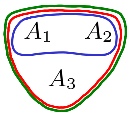
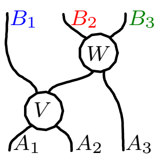
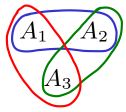
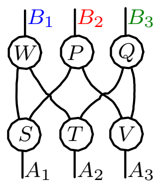
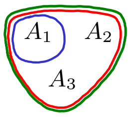
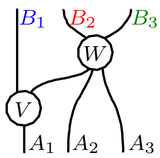
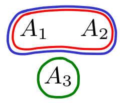
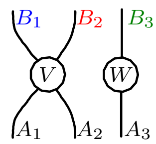
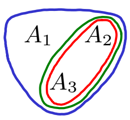
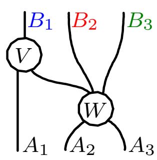
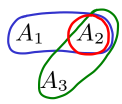
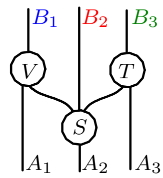
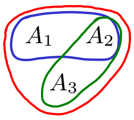
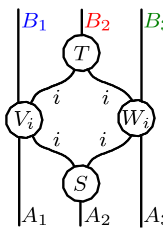
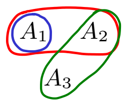
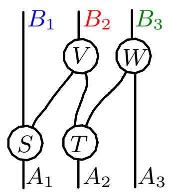
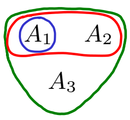
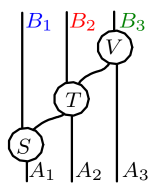
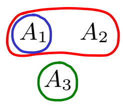
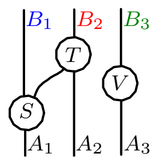


Figure 6.20: Illustration of (R2).

For type $(3,3)$ unitaries there are 17 causal structures that are inequivalent up to relabeling of the input or output systems. These are all listed in the below table, which also presents a causally faithful (extended) circuit decomposition for each case: the 5th and 11th case were covered earlier in Thm. 6.2 and Thm. 6.5, respectively, while all other cases are straightforward, either through a direct application of Thm. 6.3 or else through reduction to a known case from Secs. 6.6.1-6.6.2 via the above rules (R1)-(R4).

#	(p_1,p_2,p_3)	Causal structure	(Extended) circuit diagram	#	(p_1,p_2,p_3)	Causal structure	(Extended) circuit diagram
1	$(3,3,3)$			10	$(2,2,2)$		
2	$(3,3,2)$			11	$(2,2,2)$		
3	$(3,3,1)$			12	$(2,2,1)$		
4	$(3,2,2)$			13	$(2,2,1)$		
5	$(3,2,2)$			14	$(2,2,1)$		
6	$(3,2,1)$			15	$(2,1,1)$		

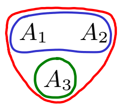
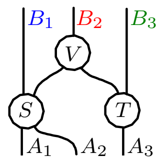
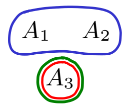
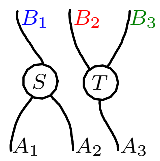
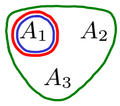
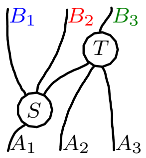
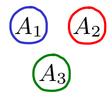
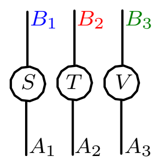
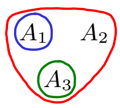
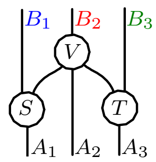
7	$(3, 2, 1)$			16	$(2, 1, 1)$		
8	$(3, 1, 1)$			17	$(1, 1, 1)$		
9	$(3, 1, 1)$						

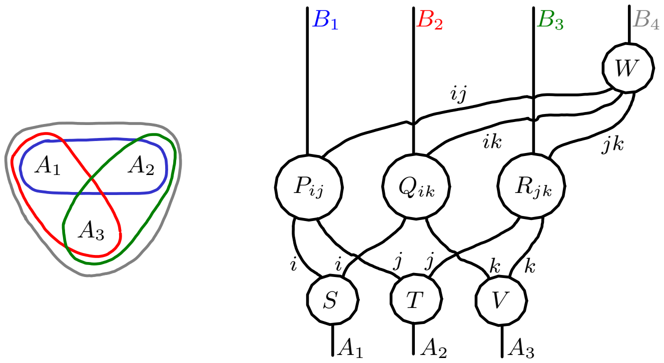
Table 6.1: List of all inequivalent causal structures, up to relabeling, of type $(3, 3)$ unitaries, together with their respective causally faithful (extended) circuit diagrams. In order to ease classification, the first column contains the tuple (p_1, p_2, p_3), where $p_1 \geq p_2 \geq p_3$ denote the cardinalities of the three parental sets in descending order. Starting with $(3, 3, 3)$ in the first row, the table progresses by considering smaller and smaller values for p_1, p_2 and p_3, making it easy to see that this is indeed the complete list of inequivalent causal structures.

6.6.4 Unitaries of type $(n, 3)$ and $(3, k)$ for $n, k \geq 4$

From now on we will not present all inequivalent causal structures up to relabeling anymore, since that becomes unfeasible and would produce little new insight. Instead we focus on those cases, where the derivation of a causally faithful extended circuit decomposition is not obvious, that is, only those cases will be presented, where an (iterative) application of the rules (R1)-(R4) does *not* straightforwardly reduce it to a simpler one.

Starting with unitaries of type $(3, k)$ for $k \geq 4$, first observe that there are only 4 distinct subsets of $\{A_1, A_2, A_3\}$ that are neither empty nor singletons. Hence, for all $k \geq 5$ the problem inevitably reduces to a simpler case due to some outputs having to have either identical parents or singleton parental sets (see (R1) and (R3)). It is only for $k = 4$ that a causal structure may exist that does not reduce to a simpler case. In fact there is only one such case, namely, the one where each of the four distinct subsets is one of the 4 parental sets. The following theorem addresses that case.

Theorem 6.6 *Given a unitary transformation* $U : \mathcal{H}_{A_1} \otimes \mathcal{H}_{A_2} \otimes \mathcal{H}_{A_3} \to \mathcal{H}_{B_1} \otimes \mathcal{H}_{B_2} \otimes \mathcal{H}_{B_3} \otimes \mathcal{H}_{B_4}$ *, if the causal structure of* U *is as in Fig. 6.21a, then* U *has a causally faithful extended circuit diagram as in Fig. 6.21b.*

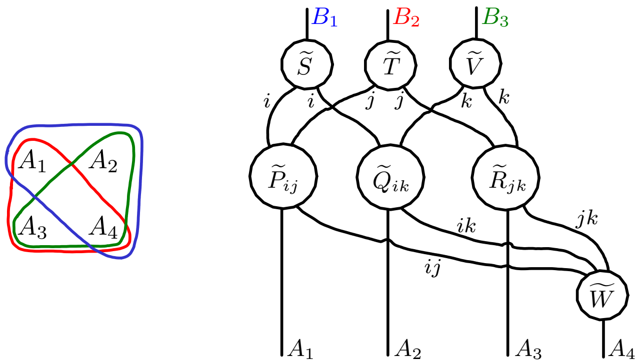


(a) (b)

Figure 6.21

Proof: See App. B.4. □

With all unitary transformations of type $(3, k)$ for $k \geq 4$ having known causally faithful extended circuit decompositions, it then follows due to Prop. 6.1 that also all unitaries of type $(n, 3)$ for $n \geq 4$ have known causally faithful extended circuit decompositions. We will therefore not explicitly treat them, with the exception of the following example of a $(4, 3)$ case. Given a unitary transformation $U : \mathcal{H}_{A_1} \otimes \mathcal{H}_{A_2} \otimes \mathcal{H}_{A_3} \otimes \mathcal{H}_{A_4} \to \mathcal{H}_{B_1} \otimes \mathcal{H}_{B_2} \otimes \mathcal{H}_{B_3}$, if the causal structure of U is as in Fig. 6.22a, then U has a causally faithful extended circuit decomposition as in Fig. 6.22b.



(a) (b)

Figure 6.22

Note that this is a prime example of a case where Prop. 6.1, i.e. in essence Thm. 6.4, is not just simplifying the classification of cases but actually doing work:

proving the above case directly does not seem straightforward, while the result is immediate by observing that the causal structure in Fig. 6.22a is dual to that in Fig. 6.21a from Thm. 6.6.

6.6.5 Unitaries of type $(4, 4)$

For unitaries of type $(4, 4)$ there exist in total 15 inequivalent causal structures that do not reduce to one of the results of the previous subsections via (R1)-(R4). For the first nine of them, depicted in Figs. 6.23-6.31, causally faithful extended circuit decompositions will be presented in the following. The remaining six cases in Figs. 6.32-6.37 will be left open.

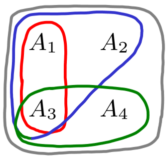


Figure 6.23

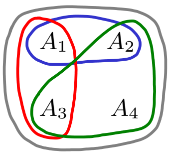


Figure 6.24

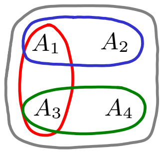


Figure 6.25

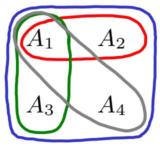


Figure 6.26

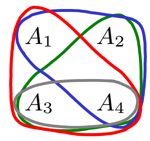


Figure 6.27

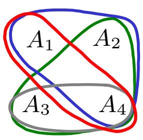


Figure 6.28

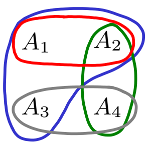


Figure 6.29

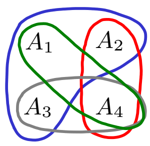


Figure 6.30

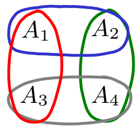


Figure 6.31

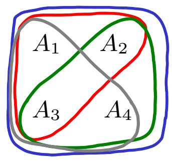


Figure 6.32

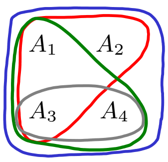


Figure 6.33

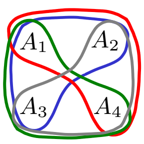


Figure 6.34

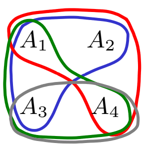


Figure 6.35

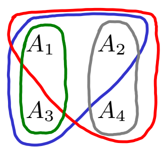


Figure 6.36

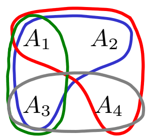


Figure 6.37

The below lemma concerns the 'nesting of indices', which was mentioned in Sec. 6.4 and which makes appearance in the subsequent Thm. 6.7 that addresses the first $(4, 4)$ case from Fig. 6.23.

Lemma 6.3 *Let* $\rho_{B_1B_2B_3|A_1A_2A_3A_4A_5} = \rho_{B_1|A_1A_3}\ \rho_{B_2|A_1A_2A_4}\ \rho_{B_3|A_1A_2A_5}$ *be the CJ representation of a channel, with the factors on the right hand side commuting pairwise.*

Then there exist a unitary S, and a family of unitaries $\{T_i\}_{i\in I}$,

$$S \;:\; \mathcal{H}_{A_1} \;\to\; \bigoplus_{i\in I} \mathcal{H}_{X_i^L} \otimes \mathcal{H}_{X_i^R} \qquad \textit{and} \qquad T_i \;:\; \mathcal{H}_{X_i^R} \otimes \mathcal{H}_{A_2} \;\to\; \bigoplus_{j_i \in J_i} \mathcal{H}_{Y_{ij_i}^L} \otimes \mathcal{H}_{Y_{ij_i}^R} \;,$$

with $\{J_i\}_{i\in I}$ a family of sets parametrized by I, such that

$$\rho_{B_1B_2B_3|A_1A_2A_3A_4A_5} \;=\; S^T \left[\bigoplus_{i\in I} \rho_{B_1|X_i^L A_3} \otimes T_i^T \left(\bigoplus_{j_i \in J_i} \rho_{B_2|Y_{ij_i}^L A_4} \otimes \rho_{B_3|Y_{ij_i}^R A_5} \right) \left(T_i^T\right)^\dagger \right] \left(S^T\right)^\dagger \;, \quad (6.6)$$

for families of channels $\{\rho_{B_1|X_i^L A_3}\}_{i\in I}$, $\{\rho_{B_2|Y_{ij_i}^L A_4}\}_{i\in I, j_i\in J_i}$ and $\{\rho_{B_3|Y_{ij_i}^R A_5}\}_{i\in I, j_i\in J_i}$.

Proof: See App. B.5. □

Theorem 6.7 *Given a unitary transformation $U : \mathcal{H}_{A_1} \otimes \mathcal{H}_{A_2} \otimes \mathcal{H}_{A_3} \otimes \mathcal{H}_{A_4} \to \mathcal{H}_{B_1} \otimes \mathcal{H}_{B_2} \otimes \mathcal{H}_{B_3} \otimes \mathcal{H}_{B_4}$, if the causal structure of U is as in Fig. 6.38a, then U has a causally faithful extended circuit diagram as in Fig. 6.38b.*

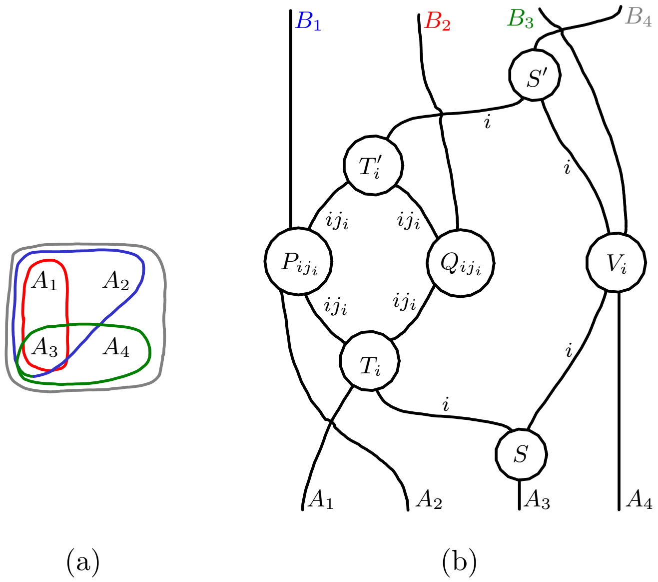
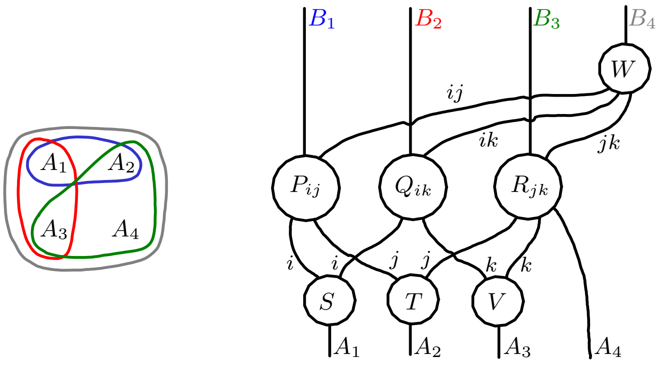


Figure 6.38

Proof: See App. B.6. □

The following three theorems present causally faithful extended circuit decompositions for the causal structures in Figs. 6.24-6.26.

Theorem 6.8 *Given a unitary $U : \mathcal{H}_{A_1} \otimes \mathcal{H}_{A_2} \otimes \mathcal{H}_{A_3} \otimes \mathcal{H}_{A_4} \to \mathcal{H}_{B_1} \otimes \mathcal{H}_{B_2} \otimes \mathcal{H}_{B_3} \otimes \mathcal{H}_{B_4}$, if the causal structure of U is as in Fig. 6.39a, then U has a causally faithful extended circuit diagram as in Fig. 6.39b.*

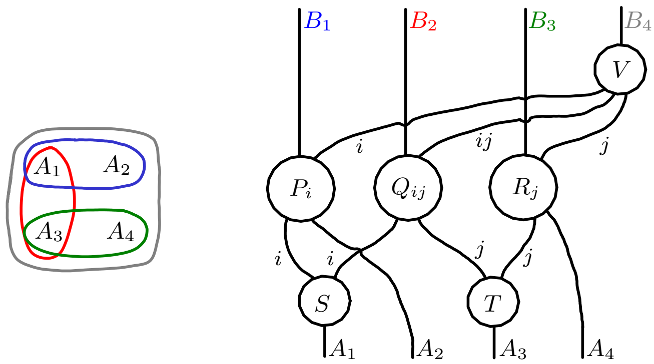


(a) (b)

Figure 6.39

Proof: See App. B.7. ☐

Theorem 6.9 *Given a unitary transformation* $U : \mathcal{H}_{A_1} \otimes \mathcal{H}_{A_2} \otimes \mathcal{H}_{A_3} \otimes \mathcal{H}_{A_4} \to \mathcal{H}_{B_1} \otimes \mathcal{H}_{B_2} \otimes \mathcal{H}_{B_3} \otimes \mathcal{H}_{B_4}$*, if the causal structure of* U *is as in Fig. 6.40a, then* U *has a causally faithful extended circuit diagram as in Fig. 6.40b.*



(a) (b)

Figure 6.40

Proof: See App. B.8. ☐

Theorem 6.10 *Given a unitary transformation* $U : \mathcal{H}_{A_1} \otimes \mathcal{H}_{A_2} \otimes \mathcal{H}_{A_3} \otimes \mathcal{H}_{A_4} \to \mathcal{H}_{B_1} \otimes \mathcal{H}_{B_2} \otimes \mathcal{H}_{B_3} \otimes \mathcal{H}_{B_4}$*, if the causal structure of* U *is as in Fig. 6.41a, then* U *has a causally faithful extended circuit diagram as in Fig. 6.41b.*

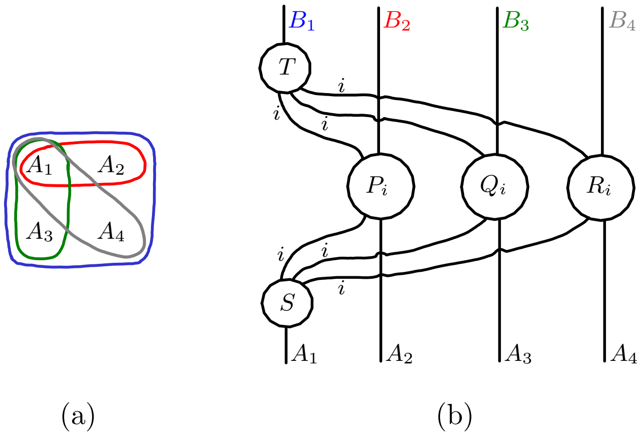


Figure 6.41

Proof: See App. B.9. □

The next two causal structures from the above list, Figs. 6.27 and 6.28, are reproduced below as Figs. 6.42 and 6.43. Observe that they are 'dual' to those in Figs. 6.24 and 6.25, addressed by Thms. 6.8 and 6.9, respectively. With Prop. 6.1 it follows that they have known causally faithful extended circuit decompositions, arising from those in Thms. 6.8 and 6.9, which will therefore not be stated explicitly.

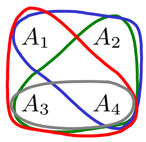


Figure 6.42

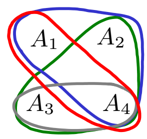


Figure 6.43

Finally, the three causal structures from Figs. 6.29-6.31 are reproduced in the below three figures, together with their respective implied causally faithful circuit decompositions. In all three cases, the proofs are analogous to that of Thm. 6.5 and hence omitted.

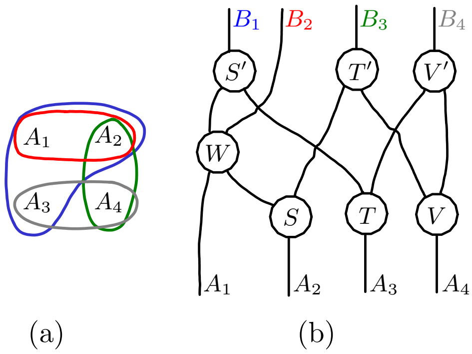


Figure 6.44: The causal structure in (a) implies a causally faithful circuit diagram as in (b).

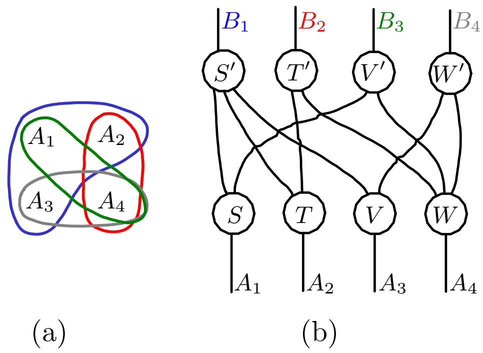


Figure 6.45: The causal structure in (a) implies a causally faithful circuit diagram as in (b).

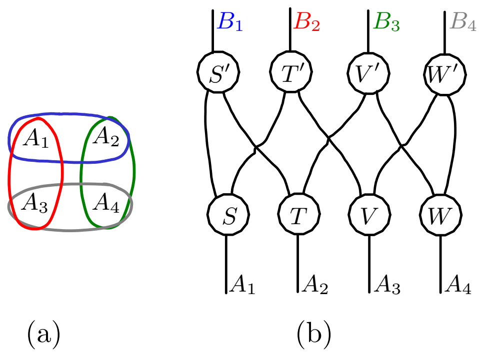


Figure 6.46: The causal structure in (a) implies a causally faithful circuit diagram as in (b).

6.7 The permissible causal structures

In light of the fact that in the previous section many causally faithful extended circuit decompositions were derived from just an assumed causal structure, one may wonder which causal structures, seen as purely combinatorial objects, are permissible at all. For any natural numbers k and n, does any choice of k non-empty subsets of a set of cardinality n, represent the causal structure of some unitary?

It is straightforward to see that the answer is 'yes' if the question is put so broadly, without any dimensional restrictions. For any choice of k subsets $Pa(B_j)$ of a set $\{A_1, ..., A_n\}$, the following is an example of a unitary $U : \mathcal{H}_{A_1} \otimes ... \otimes \mathcal{H}_{A_n} \to \mathcal{H}_{B_1} \otimes ... \otimes \mathcal{H}_{B_k}$ that instantiates that causal structure. Associate a two-dimensional Hilbert space $\mathcal{H}_{X_i^j}$ with each 'causal arrow' $A_i \in Pa(B_j)$. For each $i = 1, ..., n$ consider some unitary $V^{(i)} : \mathcal{H}_{A_i} \to \bigotimes_{j:B_j \in Ch(A_i)} \mathcal{H}_{X_i^j}$, where $Ch(A_i)$ is the set of children of A_i and similarly, for each $j = 1, ..., k$ a unitary $W^{(j)} : \bigotimes_{i:A_i \in Pa(B_j)} \mathcal{H}_{X_i^j} \to \mathcal{H}_{B_j}$.

The composition $(W^{(1)} \otimes ... \otimes W^{(k)})(V^{(1)} \otimes ... \otimes V^{(n)})$ (with suppressed swaps for well-typed composition) defines a unitary with the desired causal structure.

However, if the dimensions $d_{A_1}, ..., d_{A_n}$ and $d_{B_1}, ..., d_{B_k}$ are fixed, provided $\prod_i d_{A_i} = \prod_j d_{B_j}$ holds to allow for the existence of an invertible linear map, then in general not any causal structure is permissible.

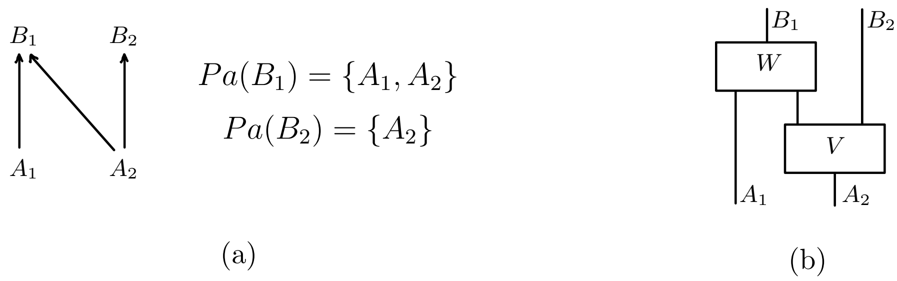


Figure 6.47: Example of a causal structure in (a) with $A_1 \nrightarrow B_2$ as the only constraint and in (b) the implied decomposition (same as Fig. 6.3a).

For instance, consider a unitary with two input and two output systems $U : \mathcal{H}_{A_1} \otimes \mathcal{H}_{A_2} \to \mathcal{H}_{B_1} \otimes \mathcal{H}_{B_2}$ and suppose its causal structure is as in Fig. 6.47a, i.e. the only causal constraint is $A_1 \nrightarrow B_2$. Then U has a circuit decomposition as in Fig. 6.47b (see, e.g., Sec. 6.2), which allows to read off dimensional restrictions on any unitary U with that causal structure: only dimensions d_{A_1}, d_{A_2}, d_{B_1} and d_{B_2} are permissible for which there exists a natural number $d \geq 2$ such that $d_{A_2} = d_{B_2}d$ and $d_{B_1} = d_{A_1}d$ hold (noting that with d being the dimension of the intermediate system, $d = 1$ would not allow causal influence from A_2 to B_1). Thus, all unitaries with the considered causal structure can be classified by triples of natural numbers (d_{A_1}, d_{B_2}, d) with $d \geq 2$.

It is a generic phenomenon that a causal structure as a combinatorial object imposes dimensional restrictions on the possible Hilbert spaces in the domain and co-domain of unitaries, which instantiate that particular causal structure. While it is in general a non-trivial question what these constraints are, for all those cases where a causally faithful extended circuit decomposition implied by the causal structure is known, then one can read off the dimensional restrictions imposed by that causal structure, just as done in the above example.

Note that one can similarly analyse the possible 'classical causal structures', taking causal relations between variables to be functional dependences in a functional model (see Sec. 3.1.2). The corresponding analogous question then concerns reversible functions $f : X_1 \times ... \times X_n \to Y_1 \times ... \times Y_k$ from n variables to k variables, each taking values in sets of finite cardinality d_{X_i} and d_{Y_j}, respectively, where the causal structure of f are the k subsets $Pa(Y_i) \subseteq \{X_1, ..., X_n\}$ of all those input variables on which Y_i functionally depends. For arbitrary natural numbers n, k, do all choices of k subsets of $\{X_1, ..., X_n\}$ appear as the causal structure of some reversible function?

By completely analogous arguments as above, just replacing tensor products with Cartesian products and unitaries with reversible functions of one's choice, the answer is 'yes' as long as the cardinalities d_{X_i} and d_{Y_j} are not fixed. Similarly does the causal structure $\{Pa(Y_i)\}_i$ in general impose 'cardinality restrictions' on the variables which can appear in the domain and co-domain of a reversible function which instantiates that causal structure. However, these constraints differ from those for unitary maps in the quantum case. Consider a reversible function $f : X_1 \times X_2 \to Y_1 \times Y_2$ and the same causal structure as in Fig. 6.47a (replacing A_i with X_i and B_i with Y_i). A concrete reversible function with that causal structure is the logical CNOT gate with X_1 as the target bit and X_2 as the control bit (CNOT is a self-inverse function). However, in this case $d_{X_2} = 2$, which is impossible to occur as the dimension of the Hilbert space $\mathcal{H}_{A_2}$ in the quantum case in Fig. 6.47. Note that the quantum CNOT gate with A_1 as the target qubit and A_2 as the control qubit is a unitary, but does not have the causal structure as in Fig. 6.47a — there is a backaction from the target qubit on the control qubit.

6.8 Decompositions of unitary processes

Given a unitary transformation $U : \mathcal{H}_{A_1} \otimes ... \otimes \mathcal{H}_{A_n} \to \mathcal{H}_{B_1} \otimes ... \otimes \mathcal{H}_{B_k}$ this chapter studied the structural consequences from its causal structure in terms of decompositions of U. Let us now return to the perspective with which this chapter started to introduce the question, namely, whether the causal mechanisms can be pinned down more precisely in a compositional manner, where the latter are 'part of' *unitary processes*. Clearly, the obtained results are completely independent from the 'physical interpretation' of U. The unitary map may be seen to describe the evolution of quantum systems $A_1, \ldots A_n$ at an earlier time to the quantum systems $B_1, \ldots, B_k$ at a later time, as is standard in physics. However, it may also be seen as a 'more abstract' unitary map U that defines a unitary process, in which case, pairs of input and output systems of the unitary map are interpreted as the output and input spaces of corresponding quantum nodes.

Recall Def. 4.7 for the concept of causal structure between the quantum nodes of a unitary process. The discussion of the cases, where this is not a DAG and extended circuit decompositions will actually turn out to facilitate new insights, is postponed to the next chapter. In order to provide the basis for these insights, here only a simple observation is made by sketching the link between extended circuit diagrams and unitary processes for when there is nothing conceptually puzzling about the latter — for *broken unitary circuits* as they were introduced in Sec. 5.2.2 (see Fig. 5.3c).

Suppose $\sigma_{A_1\dots A_n} = \rho^U_{A_1\dots A_n|A_1\dots A_n}$ is a broken unitary circuit. Furthermore, suppose the associated unitary map $U : \mathcal{H}_{A_1^{\text{out}}} \otimes \dots \otimes \mathcal{H}_{A_n^{\text{out}}} \to \mathcal{H}_{A_1^{\text{in}}} \otimes \dots \otimes \mathcal{H}_{A_n^{\text{in}}}$ has a causally faithful extended circuit decomposition. This then also yields a more fine-grained decomposition of the broken unitary circuit: seeing as $\sigma_{A_1\dots A_n}$ arises from a circuit and has a DAG as causal structure, there exists a relabeling of the quantum nodes — let this be $A_1, \dots, A_n$ — such that $A_i \nrightarrow A_j$ for all $i \geq j$ and the components of the extended circuit diagram can be appropriately 'slided around' and 'wires bent' so as to 're-identify' pairs of spaces as the corresponding quantum nodes.

Consider the following simple example as an illustration. The broken unitary circuit in Fig. 6.48b with root nodes R_1, R_2, leaf nodes L_1, L_2 and intermediate node N can be seen to arise from the unitary map $U : \mathcal{H}_{R_1} \otimes \mathcal{H}_{R_2} \otimes \mathcal{H}_{N^{\text{out}}} \to \mathcal{H}_{L_1} \otimes \mathcal{H}_{L_2} \otimes \mathcal{H}_{N^{\text{in}}}$ in Fig. 6.48d[8]. This map U is the same unitary that was already considered in Sec. 6.2 (see Fig. 6.5) and which has a causally faithful extended circuit decomposition due to Thm. 6.2. Therefore, applying the steps $(d) \to (c)$ and $(c) \to (b)$ from Fig. 6.48 to the extended circuit diagram in Fig. 6.6 yields the decomposition of the broken unitary circuit as in Fig. 6.48e.

The one no-influence relation that is not apparent from Fig. 6.48b, namely $R_1 \nrightarrow L_1$, is now evident in Fig. 6.48e through the lack of a corresponding path. More generally, causal faithfulness carries over to unitary processes in the obvious sense. If the extended circuit decomposition of U is causally faithful, then it remains the case, once wires are bent, that there is a path from node A to B in the corresponding extended circuit decomposition of the broken unitary circuit iff A is a direct cause of B.

6.9 Discussion

The main insights from this chapter can be condensed into two. First, tensor product and sequential composition do not suffice to understand causal structure of unitary transformations in compositional terms. Second, direct sum structures are

[8]As the root (leaf) nodes have a trivial input (output) space the corresponding superscript is dropped and the non-trivial spaces are just referred to as R_1 and R_2 (L_1 and L_2).

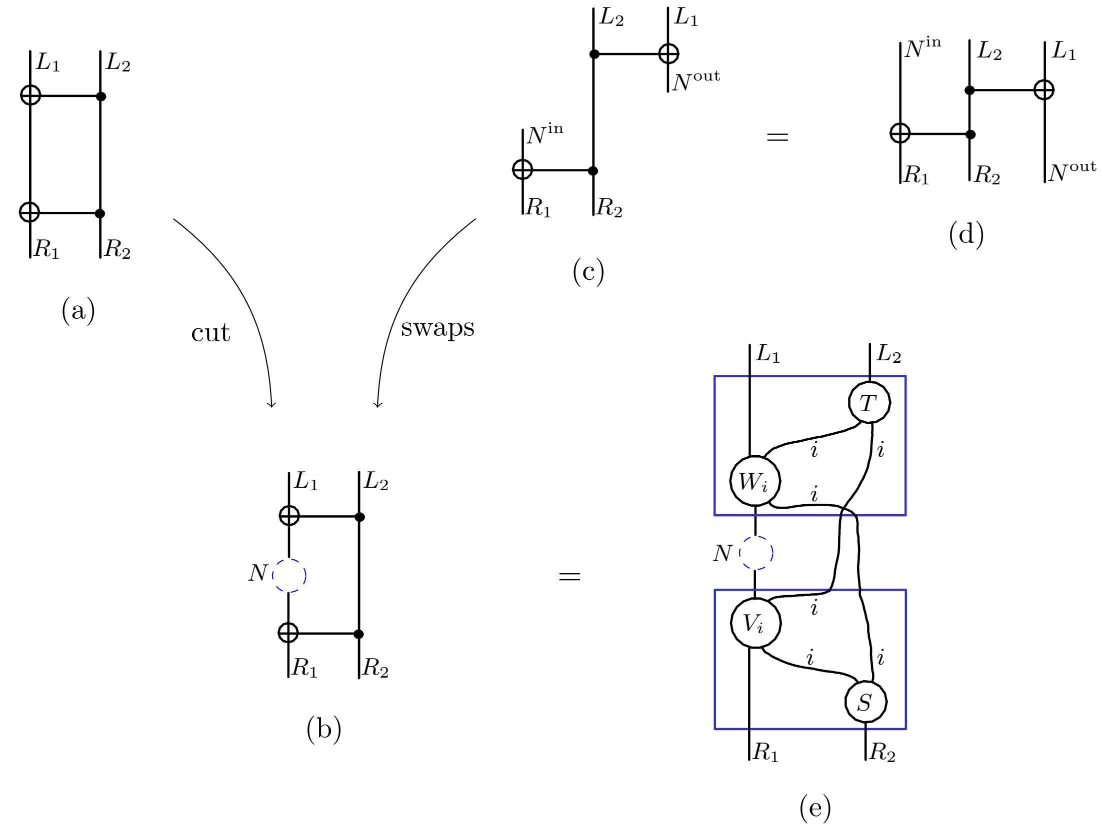


Figure 6.48: Example of a simple broken unitary circuit in (b), together with two ways of seeing how it arises – from (a) via 'breaking' wires, or from (c) via two swaps. (e) shows a causally faithful extended cirucit diagram for the broken unitary circuit.

needed in addition, which led to the introduction of extended circuit diagrams and facilitated progress by the fact that now some causal structures can be understood compositionally where this was previously impossible. In particular, causally faithful extended circuit decompositions were presented for all unitary maps of type (n, k) with arbitrary n and k at most 3, as well as arbitrary k and n at most 3. Also for a selection of causal structures of type $(4, 4)$ unitaries, causally faithful extended circuit decompositions were presented.

There are three main questions left open for future work.

The hypothesis

While the results from Sec. 6.6 lend support to Hypothesis 1, the latter remains unproven. There will be many more cases of unitaries of arbitrary type (n, k), where the same proof techniques as employed in the previous sections will allow to derive a causally faithful extended circuit decomposition. However, there are also cases where these techniques do not seem to straightforwardly allow to derive a desired decomposition, such as the six causal structures in Figs. 6.32-6.37 of type $(4,4)$ unitaries.

Note that the results in Sec. 6.6 concerning specific causal structures were all of the form that a causal structure (for a type (n,k) unitary), as a purely combinatorial object of k subsets of a set of cardinality n, implies a certain form of a causally faithful extended circuit diagram, which exists for every unitary transformation with that causal structure — completely independently from which specific unitary. Therefore, a slightly stronger version of Hypothesis 1, also supported by the presented results, is that this continues and any causal structure comes with a general causally faithful extended circuit diagram. In case that stronger version was false, it is logically conceivable that Hypothesis 1 remains valid and every particular unitary has a causally faithful extended circuit decomposition, but their forms differ among unitaries with the same causal structure.

Formalisation of the graphical language

In Sec. 6.4 *extended circuit diagrams* were introduced informally as an extension of circuit diagrams, designed to graphically express the interplay between direct sum and tensor product — not in full generality, but to the extend that this work found it to be necessary to understand causal structure compositionally.

Future work has to develop extended circuit diagrams into a formal graphical language with syntax, that is, rules of composition for the circles with indexed wires going in and out, and semantics in terms of unitary maps between finite-dimensional Hilbert spaces. To this end, it is likely to be instructive to study the precise relation between extended circuit diagrams and the work by Vicary and Reutter on *shaded tangles* (see, e.g., Refs. [145–147]), which provides a more general framework for the graphical representation of compositional structures including those expressible with extended circuit diagrams. The index sets parametrizing families of Hilbert spaces and linear maps, explicit as indices in the extended circuit diagrams here, are there represented graphically through shaded regions, leading to high-dimensional geometric objects to represent compositional structures such as in Fig. 6.8a. The works in Refs. [145–147] are not concerned with a causal analysis of linear maps and the graphical representations within their formalism of the decompositions discovered in this chapter do not necessarily achieve the purpose of rendering the causal structure visually evident, hence, the introduction of extended circuit diagrams in the first place. More generally, this future investigation will also have to study the relation to other works on graphical calculi, in particular for bimonoidal categories, (see, e.g., Refs. [21, 148]).

Extension to non-unitary channels and processes

So far, this chapter was concerned exclusively with unitary maps (and unitary processes). An obvious question is to what extent any of it can be extended beyond that.

Given a generic channel $\mathcal{C} : \mathcal{L}(\mathcal{H}_{A_1} \otimes ... \otimes \mathcal{H}_{A_n}) \to \mathcal{L}(\mathcal{H}_{B_1} \otimes ... \otimes \mathcal{H}_{B_k})$, one can still ask for each output system B_j which input systems can signal to B_j according to Def. 3.6. Let $Pa^s(B_j)$ then denote this subset of input systems that can signal to B_j. As has been emphasised throughout this thesis the sets $\{Pa^s(B_j)\}$ — merely encoding the 'single system signalling relations' — in general do not fix the channel's overall signalling structure (see, e.g., Secs. 4.1 and 5.7). A question that is analogous to the one studied here for unitary transformations, might ask after a decomposition of $\mathcal{C}$, including a graphical representation thereof, that would make its signalling structure evident through the absence and presence of paths. However, this question does not generally make sense: if A_i cannot signal to B_j and also not to B_k, the decomposition ought to reflect that through the absence of a path to either, i.e. in particular there would not be a path to the composite B_jB_k, while there however may be signalling from A_i to B_jB_k.

Now, suppose it so happens that

$$\rho^{\mathcal{C}}_{B_1...B_k|A_1...A_n} = \prod_{j=1}^{k} \rho_{B_j|Pa^s(B_j)} \ , \tag{6.7}$$

where all factors commute pairwise. First, the sets $\{Pa^s(B_j)\}$ then do determine the channel's overall signalling structure (see Sec. 5.7), making the question after a corresponding decomposition that would be 'faithful' for that signalling structure, an in principle sensible question. Second, one may furthermore hope to be able to employ the same ideas and techniques as in this chapter to find an insightful decomposition of $\mathcal{C}$ — essentially exploring when and how the decomposition obtained from the pairwise commutation relations due to Lem. 6.1 can be translated into a decomposition of $\mathcal{C}$ itself. Future work will pursue this direction further and develop a graphical language adequate to this purpose, i.e. an analogue or extension of the extended circuit diagrams to non-unitary channels.

There of course is an important class of channels, studied in detail in Chap. 5, that have the factorisation property from Eq. (6.7), namely any channel defined by the process operator of a quantum causal model (Def. 5.1)[9]. Once an appropriate analogue of extended circuit diagrams for non-unitary channels exists, one would

[9] See Rem. 5.9 for the relation between Eq. (6.7) and the parental sets defined by a causal model.

expect that the same step as described in Sec. 6.8 for unitary processes then allows to 'bend the wires' and obtain 'causal decompositions' of the non-unitary processes associated with quantum causal models.

In light of the fact that due to Thm. 5.2 Markovianity implies compatibility, given a quantum causal model involving the process $\sigma_{A_1 \ldots A_n}$, an obvious first approach would be the following. Consider the unitary process asserted to exist by virtue of compatibility of $\sigma_{A_1 \ldots A_n}$ with the causal structure of the model (cf. Def. 5.3). Suppose that unitary process has a causally faithful extended circuit decomposition in the sense as described in Sec. 6.8. If one can lift the extended circuit diagram to a representation of the channel, i.e. from the level of the underlying Hilbert spaces and linear maps to the level of CP maps, then the data which gives the marginalisation to $\sigma_{A_1 \ldots A_n}$ should allow to obtain a decomposition of the process $\sigma_{A_1 \ldots A_n}$ that now makes the causal structure of the model evident in compositional terms.

Chapter 7

Generalising quantum causal models: cyclic causal structure

This last main chapter is largely based on the third publication in Ref. [3]. It will bring together the ideas and results from all three preceding Chapters 4, 5 and 6. It will study the significance of those cases, where the causal structure of a unitary process, as defined in Def. 4.7, is a directed graph with directed cycles. In particular, it will study its significance in relation to the field of 'indefinite causal order', by bringing to the latter the causal model perspective from Chap. 5, as well as, the compositional understanding of causal structure from Chap. 6. In order to set the stage, first a brief introduction to the study of 'indefinite causal order' will be given.

7.1 Background on indefinite causal order

7.1.1 Quantum processes

One feature of quantum processes, which, amongst other reasons, made it an attractive formalism for the formulation of quantum causal models, is that it allows to represent different causal situations on an equal footing, that is, with the same kind of mathematical object. This feature was highlighted in Sec. 3.2 and is shared with other formalisms such as those in Refs. [32, 78, 79, 149]. Suppose A and B are two quantum nodes and for the sake of a more concrete discussion here, one may think of them as two labs, equipped with agents Alice and Bob who can perform interventions at A and B, respectively. A process σ_{AB} may describe a situation in which the two labs are *acausally related* and hence in particular none of the agents can signal to the other. The process σ_{AB} may also describe a situation in which they are *causally related*. Usually the presupposition is that then at most Alice can signal to Bob or vice versa, but not both — there is a causal mechanism in at most one direction. In particular if the respective labs are embedded into a fixed space-time, then space-like or time-like separation constrain which of the causal situations can obtain.

Precisely to question such presupposition and to explore the scope for possibilities, where two labs do not have a fixed causal order, while maintaining logical consistency, was the original motivation for the introduction of the process formalism by Oreshkov, Costa and Brukner (OCB) in Ref. [43]. There is a number of good reasons for such inquiry. First, could quantum theory as such be compatible with more general situations, where causal relations are 'quantum indefinite', in a sense akin to how Bell's theorem can be taken to imply the impossibility of assigning pre-existing values to observables prior to measurement. In a similar spirit Chiribella *et al.* in Ref. [42] had studied a new model of quantum computation that transcends that of quantum circuits with always a fixed causal structure, by considering higher-order quantum computations that allow to model that the connectivity of a quantum circuit itself could be controlled by the state of a quantum system and put in a superposition. Second, in the context of a search for a theory of quantum gravity it can be argued that the dynamical nature of spacetime together with the quantum phenomenon of superpositions including, say, of different spatial positions of a large mass, might lead to a dynamical causal structure as argued by Hardy [40,41] (also see [42,43,46,150] on the relevance of quantum processes to quantum gravity). Third, considering scenarios that lack a definite causal order between operations also finds motivation from studying the possibility of closed time-like curves in the context of quantum theory without ending up with non-linear modifications of the latter [42,43,46,57,58,69].

The way Oreshkov, Costa and Brukner approached the question in Ref. [43] is by deriving the general framework for describing the correlations between events in a set of labs, assuming only quantum mechanics being valid locally in the labs and the absence of logical contradictions, while in particular not assuming that there exists a fixed causal order of the labs. Suppose a set of n labs, each of which receives a system once and sends it out again, but is otherwise closed from the environment, is represented by the quantum nodes $A_1, \ldots, A_n$ and suppose $\tau_{A_1}^{k_{A_1}}, \ldots, \tau_{A_n}^{k_{A_n}}$ is a choice of local interventions. The question then becomes which probability distributions $P(k_{A_1}, \ldots, k_{A_n})$ can be obtained given the mentioned assumptions. The sense in which the standard quantum formalism is assumed to correctly describe the labs locally is two-fold. First, by virtue of considering a quantum node A with an input and an output Hilbert space and by letting local operations be represented by arbitrary quantum instruments $\{\tau_A^{k_A}\}_{k_A}$. Second, in order for convex mixtures of operations locally to give the probabilistic structure as usual, the function that maps $(\tau_{A_1}^{k_{A_1}}, \ldots, \tau_{A_n}^{k_{A_n}})$ onto $P(k_{A_1}, \ldots, k_{A_n})$ — the 'quantum process' — has to be a multilinear function, linear in all its n arguments. Requiring $P(k_{A_1}, \ldots, k_{A_n})$ to be a positive real number, also when the n labs may share any entangled auxiliary input systems amongst them, implies that the quantum process can be represented by a positive semi-definite operator $\sigma_{A_1 \ldots A_n}$ on all $2n$ Hilbert spaces:

$$P(k_{A_1}, \ldots, k_{A_n}) = \mathrm{Tr}\Big[\sigma_{A_1 \ldots A_n}\Big(\tau_{A_1}^{k_{A_1}} \otimes \ldots \otimes \tau_{A_n}^{k_{A_n}}\Big)\Big] \ . \tag{7.1}$$

The requirement that this be a correctly normalised probability distribution means that the right-hand side has to give unity for any set of local CPTP maps. Hence, the assumptions yield the formalism of process operators just as defined in Def. 3.7. See Ref. [43] for the details of the derivation (modulo our different convention for the CJ isomorphism) and see Refs. [43,48,49] for equivalent necessary and sufficient conditions for an operator to be a quantum process operator (also see Sec. C.1).

A first sense in which 'compatibility with a definite causal order' — note the different meaning compared to compatibility with a DAG from Def. 5.3 — was made precise for the bipartite case in Ref. [43] is through the notion of causal separability. A bipartite process σ_{AB} is *causally separable* if and only if it has a decomposition of the form $\sigma_{AB} = p\ \sigma_{AB}^{A \not\preceq B} + (1-p)\ \sigma_{AB}^{B \not\preceq A}$, where $0 \leq p \leq 1$ and $\sigma_{AB}^{A \not\preceq B}$ is a process, in which A cannot signal to B (cf. Def. 3.8) and $\sigma_{AB}^{B \not\preceq A}$ a process, in which B cannot signal to A. In that case σ_{AB} is a convex mixture of processes, each of which can be seen to have a fixed causal order (either summand may contain acausally related A and B). If a process σ_{AB} is not of that form it is called *causally nonseparable*.

A priori, it could have been the case that only causally separable processes exist within the framework. However, Ref. [43] presented an example of a bipartite process that is causally nonseparable, and which in subsequent works has been referred to as the *OCB process*. In fact, this process was shown to be 'incompatible with a definite causal order' in a second, stronger sense than captured by causal nonseparability. In Ref. [43] a *causal inequality* was derived that is satisfied by any bipartite correlation in a particular 'causal game' involving two agents, whenever there is a fixed causal order of their respective labs (or probabilistic mixtures thereof), regardless of any specification of what sort of systems the agents are dealing with and what the operations are they may perform. Ref. [43] then demonstrated the OCB process to violate that causal inequality. Analogously to a Bell inequality, the violation of the causal inequality certifies in a theory-independent way that the correlations could not have arisen from a fixed causal order.

Much effort has been devoted since to the exploration of the landscape of quantum processes, in particular for more than two nodes. The notion of causal separability in the multipartite case, developed by a number of works in Refs. [43,48,49,64], is not as straightforward as in the bipartite case, since one has to not only capture probabilistic mixtures of fixed causal orders, but also dynamical causal order and that causal nonseparability might be 'activated' when allowing shared entangled auxiliary input systems among the involved nodes. A formal definition is given in App. C.4 and see Refs. [49, 64] for a discussion. Many further works have studied quantum processes that can give rise to correlations that violate multipartite causal inequalities (see, e.g., Refs. [47, 49, 51, 52, 151–154]), which are, similarly to the bipartite case, incompatible with a definite causal order in a theory-independent sense [44, 49, 155]. Such processes are often referred to as 'noncausal' processes [49]. In Ref. [66] a category theoretic construction was presented that allows modelling causal structure in a general class of theories in a way that contains quantum process operators as special cases. Similarly, Ref. [67] presented a framework of higher-order quantum maps, with an operational axiomatisation thereof, that contains in particular quantum process operators as special cases.

It has been shown that access to causally nonseparable processes constitutes a resource that allows to perform certain informational tasks that are impossible if operations are required to occur in a definite causal order [44, 50, 156, 157]. One such process is the *quantum SWITCH* [42], which is the first causally nonseparable quantum process presented in the literature, in fact even before the work in Ref. [43] and the definition of multipartite causal separability. This important example of a causally nonseparable process (albeit not violating a causal inequality [44, 49]) will be discussed in some detail below in Sec. 7.4.1. Importantly, the quantum SWITCH has been implemented in a series of experiments [158–162], although the question over the precise sense in which it is a realisation of the quantum SWITCH has lead to some debate [65, 72, 83].

The maybe biggest open question of the field at this stage is which of the causally nonseparable quantum processes that exist mathematically in the framework, are also physical, i.e. can occur in nature in some sense or other. Do causal inequality violating processes exist at all? If so, maybe only in a quantum-gravitational regime? In particular the work by Araújo *et al.* in Ref. [123] made a start with tackling this question in a principled way and will feature in the subsequent discussions.

On a last note, observe that the relation between causal separability of a process σ and the properties of the induced graph G_σ (cf. Def. 5.24) is not trivial. Let σ_{AB} be a uniform mixture of a channel from A to B and vice versa, i.e. $\sigma_{AB} =$

$(1/2)\rho_{A|B}\ \rho_B + (1/2)\rho_{B|A}\ \rho_A$. This canonical example of a causally separable process has in general a graph G_σ with an arrow from A to B and conversely — it is not a DAG. What is more, in general even if G_σ is a DAG, the process may be causally nonseparable, and even noncausal.

7.1.2 Classical processes

In this thesis the formalism of quantum processes was initially presented in Sec. 3.2.3, in particular as a stage for the development of quantum causal models. It was not until Sec. 7.1.1 that the historical motivation behind quantum process operators was explained in more detail — the study of conceivable scenarios that lack a definite causal order of the operations. Similarly, Sec. 5.3 presented the definition of classical (split-node) processes, initially just as a stage to study the relation between quantum and classical causal models. This is the reason why a classical split node was presented as the classical analogue of a quantum $\imath$node, that is, the variables X^{in} and X^{out} were assumed to be copies of each other. This ensured an unambiguous transition to a picture with a single variable per node and a probability distribution over them to link with classical causal models. This also explains the terminology of a classical *split* node for disambiguation.

In contrast, now the focus is to appreciate the original interest in the formalism of classical processes as introduced by Baumeler, Feix and Wolf in Ref. [47] — the study of the analogous question to the quantum case, namely, what are the logically consistent classical processes that lack a definite causal order. The variables X^{in} and X^{out} of a classical (split) node X may now take values in arbitrary sets of finite cardinality. It of course maintains to be the case that classical processes $\kappa_{X_1 \ldots X_n}$ over classical nodes $X_1, \ldots, X_n$ can be seen as a special case of quantum processes in the sense of the inductions $I_{\kappa\to\sigma}$ and $I_{\sigma\to\kappa}$, only now for arbitrary nodes.

For only two nodes the original OCB paper in Ref. [43] had already looked at the classical special case of quantum processes. It found that all bipartite classical processes κ_{XY} over two classical split nodes X and Y are all convex mixtures of at most X can signal to Y and the converse. This is what one might have expected — nothing exotic in a fundamentally classical set-up. The more surprising it was that Ref. [47] found that classical processes over more than two nodes, in fact as few as three nodes, exist that are not compatible with any fixed causal order of the classical nodes. Further detailed study of classical processes followed in, e.g., Refs. [52,58,69]. This can be seen as crucial work to help understand what it is about causally nonseparable quantum processes that is due to the quantum nature of systems and what is due to the general assumptions — or lack thereof — in the process formalism and similarly conceiveable in a purely classical set-up. Independently from that perspective, in particular closed time-like curves have provided motivation for the study of classical processes without a definite causal order [47, 52, 58, 69].

Let us briefly mention some of the findings in the literature that are relevant to later discussions in Sec. 7.6. Just as in Sec. 5.3, we let a classical process interchangeably refer to the classical process map $\kappa_{X_1 \ldots X_n}$ as in Def. 5.5 (modulo arbitrary input and output variables now), to the quantum process operator diagonal in a preferred basis and the associated channel $P(X_1^{\text{in}}, ..., X_n^{\text{in}} | X_1^{\text{out}}, ..., X_n^{\text{out}})$. A classical process $\kappa_{X_1 \ldots X_n}$ over classical nodes $X_1, \ldots, X_n$ is called a *deterministic* process if and only if there exists a function $f : X_1^{\text{out}} \times .... \times X_n^{\text{out}} \to X_1^{\text{in}} \times .... \times X_n^{\text{in}}$ such that

$$P(X_1^{\text{in}}, ..., X_n^{\text{in}} | X_1^{\text{out}}, ..., X_n^{\text{out}}) = \delta((X_1^{\text{in}}, ..., X_n^{\text{in}}), f(X_1^{\text{out}}, ..., X_n^{\text{out}})) \ . \tag{7.2}$$

A deterministic process will often be denoted as $\kappa^f_{X_1 \ldots X_n}$. When f is bijective, the deterministic process is called *reversible*.

As was shown in Ref. [52], the set of classical processes over nodes $X_1, ..., X_n$ forms a polytope. The same work also showed that the *deterministic polytope*, defined by the set of deterministic processes as the set of vertices, is generally a strict subset of the polytope of all classical processes. Furthermore, Ref. [52] showed that there even exist deterministic processes that are incompatible with a definite causal order (see Sec. 7.4.2 for an example).

7.2 Generalised quantum causal models

7.2.1 The idea

The very conception of the process formalism in Ref. [43] and the interest in causally nonseparable processes are, above all, motivated from foundational questions that are phrased in causal terms — seeking to understand the most general 'causal situation' admissible in nature. At the same time, there is no framework that allows to maintain a principled way of enquiring about causal explanations of causally nonseparable processes. However, the development of such, provided possible, seems highly desirable. Not only as a matter of principle just as in the acyclic case, but one might hope that the development of such a framework actually facilitates progress with some of the technical questions of the field.

It is thus natural to wonder whether the causal model perspective can be brought to the study of causally nonseparable processes. In particular, a question, which was already formulated by Costa and Shrapnel in Ref. [82], concerns what the relation between indefinite causal order and cyclic directed graphs is. However, so far no general enough causal model framework has been proposed to answer such questions. Although Ref. [82] raised the question, the definition of a quantum causal model that work is based on, does not allow for a straightforward extension. Similarly in a causal model context, also Ref. [83] considered the idea of causal explanations in terms of directed cycles, however, to then dismiss such a possibility for reasons of conflict with their notion of 'autonomy of causal mechanisms'.

The following presents a generalised framework of quantum causal models by extending the one from Chap. 5 to cyclic causal structures. This will go in the obvious way, namely, by simply allowing for directed graphs, rather than only directed acyclic graphs, seeing as much of the concepts defined in Secs. 5.1 and 5.2 naturally suggest such a generalisation. It is almost as if we previously had to explicitly suppress this generality for the sake of a conceptually clear journey — it was a matter of first 'sanity-checking' the approach to quantum causal models in the acyclic case, that is, testing it against the conventional, well-understood part of the quantum formalism. Thus gained confidence in the approach through the results in Chap. 5, now the goal is to learn something new about the exotic, less understood processes by employing the fully general definition of causal structure of a unitary process in Def. 4.7.

7.2.2 The definition

The following definition generalises Def. 5.1, by essentially dropping the condition of acyclicity for the causal structure.

Definition 7.1 (Quantum causal model — generalized): *A* Quantum causal model *is given by:*

(1) *a causal structure represented by a directed graph G with vertices corresponding to quantum nodes $A_1, ..., A_n$,*

(2) *for each A_i, a quantum channel $\rho_{A_i|Pa(A_i)} \in \mathcal{L}(\mathcal{H}_{A_i^{in}} \otimes \mathcal{H}^*_{Pa(A_i)^{out}})$ such that $[\rho_{A_i|Pa(A_i)}\ ,\ \rho_{A_j|Pa(A_j)}] = 0$ for all i,j and such that $\sigma_{A_1...A_n} = \prod_i \rho_{A_i|Pa(A_i)}$ is a process operator over the quantum nodes $A_1, ..., A_n$.*

A directed graph that contains at least one directed cycle will be referred to as a *cyclic directed graph*. Similarly a *cyclic quantum causal model* is one whose causal structure is cyclic. Otherwise, it is called an *acyclic quantum causal model* to specifically refer to the special case according to Def. 5.1. It is understood implicitly throughout that a directed graph has *no directed one-cycle*, i.e. no arrows from a node A to itself.

Also the Markov condition from Def. 5.2 generalises, so that a quantum causal model can be referred to as the pair $(G, \sigma_{A_1 \dots A_n})$ with G a directed graph with vertices $A_1, \dots, A_n$ and $\sigma_{A_1 \dots A_n}$ a process that is Markov for G.

Definition 7.2 (Quantum Markov condition — generalized): *Given a directed graph G, with vertices corresponding to the quantum nodes $A_1, \dots, A_n$, a process $\sigma_{A_1 \dots A_n}$ is called* Markov *for G if and only if it admits a factorization into pairwise commuting channels of the form $\sigma_{A_1 \dots A_n} = \prod_{i=1}^n \rho_{A_i|Pa(A_i)}$.*

As observed in Rem. 5.1, it is trivially the case that a product of pairwise commuting operators of the form $\prod_i \rho_{A_i|Pa(A_i)}$ is a process if the parental sets $Pa(A_i)$ form a DAG. In contrast, for a cyclic directed graph this is a non-trivial condition and hence an explicit requirement in the above Def. 7.1 — it is what ensures the absence of logical paradoxes despite the apparent causal cycles.

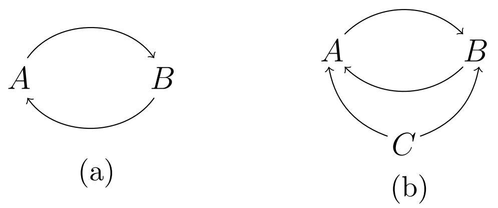


Figure 7.1: Examples of cyclic directed graphs.

Consider for instance a bipartite scenario with two nodes A and B. The unique cyclic directed graph G is depicted in Fig. 7.1a. Suppose a QCM has G as its causal structure, it then comes with a process operator of the form

$$\sigma_{AB} \;=\; \rho_{A|B}\,\rho_{B|A}\;. \tag{7.3}$$

If, however, both $\rho_{A|B}$ and $\rho_{B|A}$ are signalling channels, then σ_{AB} could not be a process operator, as loosely speaking, there would exist interventions at A and B, which led to a contradiction for their outcomes. To state this more formally and succinctly, first note that the notion of faithfulness of a quantum causal model from Sec. 5.7.3 straightforwardly generalises: a quantum causal model $(G, \sigma_{A_1 \dots A_n})$ is called *faithful* if and only if for each $i = 1, \dots, n$ the channel $\rho_{A_i|Pa(A_i)}$ allows signalling to A_i^{in} from each of the parents' output spaces[1].

[1]Equivalently, $(G, \sigma_{A_1 \dots A_n})$ is faithful if and only if $G = G_\sigma$ for the induced graph G_σ as defined in Sec. 5.7.1.

Proposition 7.1 *There is no faithful cyclic quantum causal model with two nodes.*

Proof. See App. C.2. □

Now consider a scenario with three nodes A, B and C with a causal structure G as in Fig. 7.1b. A corresponding QCM comes with a process operator of the form

$$\sigma_{ABC} = \rho_{A|BC}\ \rho_{B|AC}\ \rho_C\ . \tag{7.4}$$

While the cycle from Fig. 7.1a, which on its own does not accommodate a faithful bipartite QCM, is a subgraph of G, there now are faithful tripartite QCMs of the form as in Eq. (7.4) with G as causal structure (see Sec. 7.4 for a concrete example). The crucial difference between Eq. (7.3) and Eq. (7.4) is that in the latter the non-trivial action of the two operators $\rho_{A|BC}$ and $\rho_{B|AC}$ overlaps on C^{out} — it is essentially the decomposition of the operators thereby implied due to Lem. 4.1 that will allow to understand how it is possible to have signalling from A to B, as well as conversely, without leading to contradictions.

A first conclusion thus is that in contrast to DAGs, where every possible DAG accommodates a faithful QCM, not all cyclic directed graphs accommodate a faithful QCM. Moreover, note that even given a cyclic graph G that does accommodate some faithful cyclic QCM, it is not true that any set of pairwise commuting operators $\{\rho_{A_i|Pa(A_i)}\}$ defines a process operator by considering their product (see App. C.3 for an explicit example).

7.3 Cyclic causal structure and the Markov condition

7.3.1 Compatibility with a directed graph

Chapter 4 presented in Def. 4.7 the general notion of causal structure of a unitary process, representable as a directed graph that may contain directed cycles. Just as with acyclic quantum causal models the idea is that the directed graph that is part of a QCM is a candidate causal structure as the property that pertains to the actual underlying unitary process.

Due to Thm. 4.1 it is immediate that any unitary process $\sigma_{A_1\ldots A_n}$ together with its causal structure G defines a faithful quantum causal model, in particular if G is cyclic. In order to make precise what the relation between non-unitary processes and causal structure is, the below will follow the same ideas as in the acyclic case in Sec. 5.2.1, that is, spell out what the notion of *compatibility with a directed graph* is. It is instructive to first define the following property, which was introduced by Araújo *et al.* in Ref. [123][2].

Definition 7.3 (Unitary extendibility) [123]: *A process $\sigma_{A_1\ldots A_n}$ is called* unitarily extendible *if and only if there exists a unitary process $\sigma_{A_1\ldots A_n PF} = \rho^{\mathcal{U}}_{A_1\ldots A_n F|A_1\ldots A_n P}$ on the quantum nodes $A_1, \ldots, A_n$, plus additional root node P and leaf node F, such that $\sigma_{A_1\ldots A_n} = \mathrm{Tr}_{FP}[\sigma_{A_1\ldots A_n PF}\ \tau_P]$ for some state $\tau_P \in \mathcal{L}(\mathcal{H}^*_{P^{out}})$. The process $\sigma_{A_1\ldots A_n PF}$ is called a* unitary extension *of $\sigma_{A_1\ldots A_n}$.*

A major discovery from Ref. [123] is that not all processes are unitarily extendible. While every process, seen as a channel from the output spaces to the input spaces of all nodes, has a dilation to a unitary channel, this channel will generally not define a process. A discussion of the original motivation for presenting the above notion in Ref. [123] is postponed to Sec. 7.8.

The same arguments as discussed in Sec. 5.2.1 concerning what one should care about when calling a process $\sigma_{A_1\ldots A_n}$ compatible with a certain DAG G as causal structure — that is, no need for additional common causes in an underlying unitary process from which $\sigma_{A_1\ldots A_n}$ may be seen to arise — now naturally lead to the following analogous concept for directed graphs.

Definition 7.4 (Compatibility with a directed graph): *A process $\sigma_{A_1\ldots A_n}$ is* compatible *with a directed graph G with nodes $A_1, ..., A_n$, iff $\sigma_{A_1\ldots A_n}$ is extendible to a unitary process $\sigma_{A_1\ldots A_n\lambda_1\ldots\lambda_n F}$, with an extra root node λ_i for $i = 1, ..., n$ and an extra leaf node F, such that:*

1. *there exists a product state $\tau_{\lambda_1}\otimes\cdots\otimes\tau_{\lambda_n}$ with $\tau_{\lambda_i} \in \mathcal{L}(\mathcal{H}^*_{\lambda_i^{out}})$ such that $\sigma_{A_1\ldots A_n} = \mathrm{Tr}_{\lambda_1\ldots\lambda_n F}\left[\ \sigma_{A_1\ldots A_n\lambda_1\ldots\lambda_n F}\ (\tau_{\lambda_1}\otimes\cdots\otimes\tau_{\lambda_n})\right]$,*
2. *$\sigma_{A_1\ldots A_n\lambda_1\ldots\lambda_n F}$ satisfies the following no-influence conditions (with $Pa(A_i)$ referring to G): $\{A_j \nrightarrow A_i\}_{A_j\notin Pa(A_i)}$, $\{\lambda_j \nrightarrow A_i\}_{j\neq i}$.*

Note that in the acyclic case, Thm. 5.1 established that the unitary process asserted to exist by virtue of compatibility with a DAG G, has a realisation as a broken unitary circuit. This filled the gap between the abstract unitary process and what we understand to be, at least in principle, physically realisable. In case of compatibility with a cyclic directed graph, it clearly cannot have a circuit realisation. However, seeing as it is generally not understood yet what the criterion for physical

[2] Therein the property from Def. 7.3 is referred to as purifiability and a unitary extension is called a purification. The reason for the deviation in terminology here is that a 'purification' could naturally be understood as an extension to an isometric process, i.e. to one where the channel defined by the process is an isometric channel.

realisability for (causally nonseparable) processes should be, it is not clear what a theorem to an analogous effect to that of Thm. 5.1 should establish in the cyclic case.

7.3.2 The conjecture

Concerning acyclic causal structures, the main result from Sec. 5.2.3 established equivalence between compatibility with a DAG and Markovianity for that DAG. Concerning cyclic causal structures, one direction is straightforward.

Theorem 7.1 *If a process $\sigma_{A_1 \ldots A_n}$ is compatible with the directed graph G, then it is also Markov for G.*

Proof. Completely analogous to the proof of '(1) → (2)' of Thm. 5.2 and essentially a consequence of Thm. 4.1. For the sake of completeness: the unitary extension, asserted to exist by virtue of the assumed compatibility with G, has to factorize into pairwise commuting operators of the form $\sigma_{A_1 \ldots A_n \lambda_1 \ldots \lambda_n F} = \rho_{F|A_1 \ldots A_n \lambda_1 \ldots \lambda_n} \left(\prod_i \rho_{A_i|Pa(A_i)\lambda_i} \right)$. This yields $\sigma_{A_1 \cdots A_n} = \prod_i \mathrm{Tr}_{\lambda_i} \left[\ \rho_{A_i|Pa(A_i)\lambda_i} \ \tau_{\lambda_i} \ \right]$, where the factors $\rho_{A_i|Pa(A_i)} := \mathrm{Tr}_{\lambda_i} \left[\ \rho_{A_i|Pa(A_i)\lambda_i} \ \tau_{\lambda_i} \right]$ are pairwise commuting operators. □

The converse direction does not seem as straightforward. Given a process $\sigma_{A_1 \ldots A_n}$ that is Markov for a directed graph G, the same steps as in the proof of Thm. 5.2 guarantee the existence of a unitary channel with the appropriate causal constraints, i.e. no additional common causes are introduced. However, it is not obvious that this unitary channel can also be chosen such that it defines a unitary process. We leave this as a conjecture.

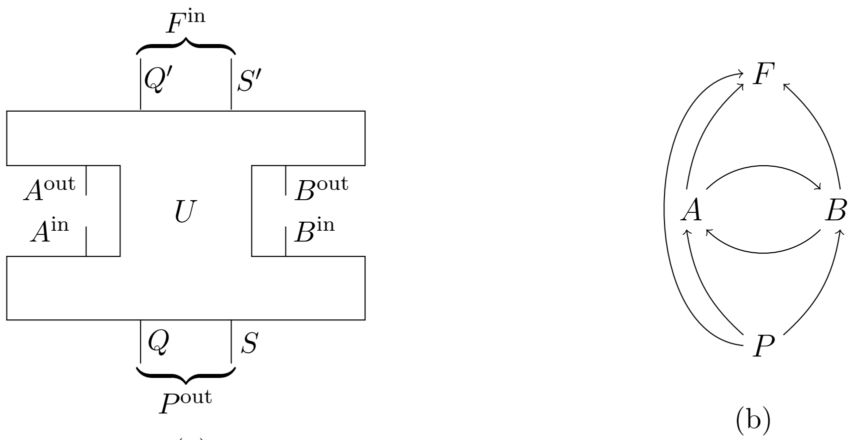
Conjecture 1 *If a process $\sigma_{A_1 \ldots A_n}$ is Markov for a directed graph G, then it is compatible with G.*

A discussion of the consequences from the validity or invalidity of the conjecture is postponed to Sec. 7.7. The next section will present a couple of concrete examples of faithful cyclic QCMs.

7.4 Examples of cyclic quantum causal models

7.4.1 The quantum SWITCH

The first example of a causally nonseparable process described in the literature is the quantum SWITCH [42]. It is typically presented as a higher-order map [32, 42, 67],



(a) (b)

Figure 7.2: The quantum SWITCH in (a) with its causal structure G_{SWITCH} in (b).

which maps pairs of CP maps of the types $\mathcal{F}_A : \mathcal{L}(\mathcal{H}_{A^{\text{in}}}) \to \mathcal{L}(\mathcal{H}_{A^{\text{out}}})$ and $\mathcal{G}_B : \mathcal{L}(\mathcal{H}_{B^{\text{in}}}) \to \mathcal{L}(\mathcal{H}_{B^{\text{out}}})$ with $d_{A^{\text{in}}} = d_{A^{\text{out}}} = d_{B^{\text{in}}} = d_{B^{\text{out}}} = d$, to a CP map of the type $\mathcal{E} : \mathcal{L}(\mathcal{H}_Q \otimes \mathcal{H}_S) \to \mathcal{L}(\mathcal{H}_{Q'} \otimes \mathcal{H}_{S'})$ with $d_Q = d_{Q'} = 2$ and $d_S = d_{S'} = d$. The basic idea is that a control qubit, which is represented by $\mathcal{H}_Q$ and $\mathcal{H}_{Q'}$ at an initial and a final time, controls in a coherent manner in which order the maps $\mathcal{F}_A$ and $\mathcal{G}_B$ act on a target system S, which is represented by $\mathcal{H}_S$ and $\mathcal{H}_{S'}$ at the initial and final time.

For our purpose it is convenient to give a precise definition of the quantum SWITCH by seeing the higher-order map as a quantum process over four nodes as depicted in Fig. 7.2a: the nodes A and B are the slots where $\mathcal{F}_A$ and $\mathcal{G}_B$ are inserted, the node P in the 'past' with $\mathcal{H}_{P^{\text{out}}} = \mathcal{H}_Q \otimes \mathcal{H}_S$ is where the control qubit and target system are initially prepared in a state, and finally the node F in the 'future' with $\mathcal{H}_{F^{\text{in}}} = \mathcal{H}_{Q'} \otimes \mathcal{H}_{S'}$ is where the control qubit and target system can be measured at the final time. The quantum SWITCH is then given by the unitary process

$$\sigma^{\text{SWITCH}}_{ABPF} = \rho^U_{ABF|ABP} = |W\rangle\langle W| \ , \quad \text{where} \tag{7.5}$$

$$\begin{aligned} |W\rangle := \ & |0\rangle_{Q^*} |0\rangle_{Q'} |\phi^+\rangle_{S^* A^{\text{in}}} |\phi^+\rangle_{(A^{\text{out}})^* B^{\text{in}}} |\phi^+\rangle_{(B^{\text{out}})^* S'} \\ & + |1\rangle_{Q^*} |1\rangle_{Q'} |\phi^+\rangle_{S^* B^{\text{in}}} |\phi^+\rangle_{(B^{\text{out}})^* A^{\text{in}}} |\phi^+\rangle_{(A^{\text{out}})^* S'} \ , \end{aligned} \tag{7.6}$$

with $|\phi^+\rangle_{XY} := \sum_i |i\rangle_X |i\rangle_Y$.

It is not hard to check that the causal structure of $\sigma^{\text{SWITCH}}_{ABPF}$ is given by the cyclic directed graph G_{SWITCH} in Fig. 7.2b. As pointed out in Sec. 7.3.1, as a unitary process, $\sigma^{\text{SWITCH}}_{ABPF}$ together with G_{SWITCH} forms a faithful cyclic quantum causal model:

$$\sigma^{\text{SWITCH}}_{ABPF} = \rho_{F|ABP} \ \rho_{A|BP} \ \rho_{B|AP} \ \rho_P \ . \tag{7.7}$$

Here ρ_P appears explicitly to emphasise Markovianity for G_{SWITCH}, although ρ_P is equal to the real number one, seeing as P^{in} is trivial. Note that also if introducing a non-trivial input space P^{in}, the above data would of course still define a faithful cyclic QCM for an arbitrary state ρ_P.

Finally, consider the (causally separable) marginal process $\sigma_{ABP} = \text{Tr}_F\left[\sigma^{\text{SWITCH}}_{ABPF}\right]$ on three nodes. It follows from Eq. (7.7) that $\sigma_{ABP} = \rho_{A|BP}\ \rho_{B|AP}\ \rho_P$ and, hence, σ_{ABP} together with the directed graph from Fig. 7.1b (relabeling C as P) forms a faithful cyclic quantum causal model, too. This establishes the claim from Sec. 7.2.2 that such tripartite QCMs exist.

7.4.2 A causal inequality violating process — the AF process

The quantum SWITCH was presented above as an example of a causally nonseparable process that can be understood as a quantum causal model with cyclic causal structure. However, it does not violate any causal inequality; it is not a noncausal process. As pointed out in Sec. 7.1, noncausal processes give rise to correlations in the outcome statistics that are not explicable with any causally separable process, no matter how large the input and output systems at the nodes or of what kind they are. They are therefore regarded genuinely incompatible with any causal order of the nodes and the immediate question is whether cyclic quantum causal models exist that involve processes of that kind. It turns out that such models do exist.

A well-known example of a noncausal process is the tripartite process discovered by Araújo and Feix (AF) and first published and further studied by Baumeler and Wolf in Ref. [52, 163].[3] It is a deterministic classical process (see Sec. 7.1.2) and yet noncausal. Here it will be convenient to present it as a special case of a quantum process operator that is diagonal with respect to a product basis of orthonormal bases for all involved input and output spaces. Let A, B and C be quantum nodes with two-dimensional input and output systems. The AF process is then given by the following process operator.

$$\sigma^{\text{AF}}_{ABC} = \rho_{A|BC}\ \rho_{B|CA}\ \rho_{C|AB},$$

where

$$\rho_{A|BC} \;=\; \sum_{b,c=0,1} |\neg b \wedge c\rangle\langle \neg b \wedge c|_{A^{\text{in}}} \otimes |b,c\rangle\langle b,c|_{(B^{\text{out}}C^{\text{out}})^*},$$

[3] See Ref. [52], where M. Araújo and A. Feix are acknowledged for the discovery of this process.

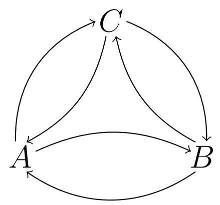


Figure 7.3: The causal structure of the AF process[4].

$$\rho_{B|CA} = \sum_{c,a=0,1} |\neg c \wedge a\rangle\langle \neg c \wedge a|_{B^{\text{in}}} \otimes |c,a\rangle\langle c,a|_{(C^{\text{out}}A^{\text{out}})^*},$$
$$\rho_{C|AB} = \sum_{a,b=0,1} |\neg a \wedge b\rangle\langle \neg a \wedge b|_{C^{\text{in}}} \otimes |a,b\rangle\langle a,b|_{(A^{\text{out}}B^{\text{out}})^*}.$$

It is evident that σ^{AF}_{ABC} is Markov for the cyclic directed graph G in Fig. 7.3, seeing as the operators, all diagonal in the same basis, commute trivially. It is also easy to see that each arrow in Fig. 7.3 corresponds to a direct signalling relation, and hence, the pair of σ^{AF}_{ABC} and G constitutes a faithful cyclic quantum causal model.

For this process to be in keeping with Conjecture 1, it had better be compatible with G. Baumeler and Wolf (BW) [163] showed that σ^{AF}_{ABC} is unitarily extendible to the following unitary extension (also see Refs. [57, 123]):

$$\sigma^{\text{BW}}_{ABCFP} = \rho^{U}_{ABCF|ABCP}\ , \tag{7.8}$$

where the additional root node P has a tensor product of three qubits as its output space, $\mathcal{H}_{P^{\text{out}}} = \mathcal{H}_{\lambda_A} \otimes \mathcal{H}_{\lambda_B} \otimes \mathcal{H}_{\lambda_C}$, and the corresponding unitary map U is defined by the following bijection of orthonormal bases:

$$\begin{aligned} U \ : \ & |a,b,c\rangle_{A^{\text{out}}B^{\text{out}}C^{\text{out}}} \ \otimes \ |i,j,k\rangle_{\lambda_A\lambda_B\lambda_C} \ \mapsto \\ & |i \oplus (\neg b \wedge c),\ j \oplus (\neg c \wedge a),\ k \oplus (\neg a \wedge b)\rangle_{A^{\text{in}}B^{\text{in}}C^{\text{in}}} \ \otimes \ |a,b,c\rangle_{F^{\text{in}}}\ . \end{aligned} \tag{7.9}$$

The AF process is recovered from $\sigma^{\text{BW}}_{ABCFP}$ if tracing F and feeding in the product state $|0,0,0\rangle$ for λ_A, λ_B and λ_C. Finally, it is not hard to check that the causal structure of the unitary process $\sigma^{\text{BW}}_{ABCFP}$ is as depicted in Fig. 7.4, i.e. it is given by the graph that arises from that in Fig. 7.3 if adding arrows from everywhere to the additional node F and arrows from λ_X to X and F for $X = A, B, C$. The BW extension therefore has the appropriate properties to establish compatibility of

[4]Strictly speaking, as a non-unitary quantum process, σ^{AF}_{ABC} does not *have* a causal structure, however, as a classical deterministic process it does (see Sec. 7.6.2). Also note that the directed graph in Fig. 7.3 is the induced graph G_σ when seeing σ^{AF}_{ABC} as a quantum process.

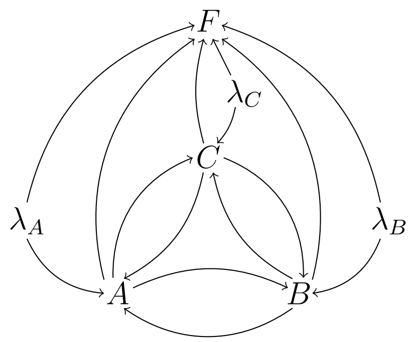


Figure 7.4: The causal structure of the BW extension of the AF process.

σ^{AF}_{ABC} with the cyclic directed graph G in Fig. 7.3.

7.5 Cyclicity and extended circuit decompositions

Recall the undertaking in Chapter 6 that studied the structural consequences for unitary transformations ensuing from causal constraints, in order to answer the question whether causal structure can be understood in compositional terms through extended circuit diagrams. Section 6.8 observed that if the unitary map U that corresponds to the unitary process $\sigma_{A_1\ldots A_n} = \rho^U_{A_1\ldots A_n|A_1\ldots A_n}$ given by a broken unitary circuit, has a (causally faithful) extended circuit decomposition, then by 'sliding components of the diagram around' one can obtain a corresponding decomposition of the unitary process. See the example in Fig. 6.48. Note that nothing about this observation relied on the acyclicity of the process' causal structure and the naturally arising question is which insights can be gained from studying such decompositions for unitary processes with cyclic causal structures. Because Hypothesis 1 remains unproven and causally faithful extended circuit decompositions are not (yet) known for all unitary transformations at the time of writing, this question cannot be answered in full generality. However, the following two examples show that this is a fruitful and promising approach to the study of causally nonseparable processes.

7.5.1 Looking inside the quantum SWITCH

The quantum SWITCH seen as a unitary process on four nodes, $\sigma^{\text{SWITCH}}_{ABPF} = \rho^{\mathcal{U}}_{ABF|ABP}$, is given by Eqs. (7.5) and (7.6). It defines a corresponding unitary map $U : \mathcal{H}_{A^{\text{out}}} \otimes \mathcal{H}_{P^{\text{out}}} \otimes \mathcal{H}_{B^{\text{out}}} \to \mathcal{H}_{A^{\text{in}}} \otimes \mathcal{H}_{F^{\text{in}}} \otimes \mathcal{H}_{B^{\text{in}}}$, which is depicted in Fig. 7.5 together with the two causal constraints as ruled by the process' causal structure from Fig. 7.2b.

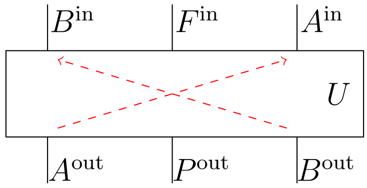


Figure 7.5: The unitary map U defined by the quantum SWITCH and, in red, the two causal constraints U satisfies.

Thus, this unitary U is precisely of the kind treated in Sec. 6.3 and due to Thm. 6.2 has a causally faithful extended circuit decomposition of the following form:

$$U = \left(\mathbb{1}_{B^{\mathrm{in}}} \otimes T \otimes \mathbb{1}_{A^{\mathrm{in}}}\right)\left(\bigoplus_{i\in I} V_i \otimes W_i\right)\left(\mathbb{1}_{A^{\mathrm{out}}} \otimes S \otimes \mathbb{1}_{B^{\mathrm{out}}}\right) , \tag{7.10}$$

where S and T are unitaries, and $\{V_i\}_{i\in I}$ and $\{W_i\}_{i\in I}$ families of unitaries of the form

$$\begin{aligned}
S &: \mathcal{H}_{P^{\mathrm{out}}} \to \bigoplus_{i\in I} \mathcal{H}_{X_i^L} \otimes \mathcal{H}_{X_i^R} , \\
V_i &: \mathcal{H}_{A^{\mathrm{out}}} \otimes \mathcal{H}_{X_i^L} \to \mathcal{H}_{Y_i^L} \otimes \mathcal{H}_{B^{\mathrm{in}}} , \\
W_i &: \mathcal{H}_{X_i^R} \otimes \mathcal{H}_{B^{\mathrm{out}}} \to \mathcal{H}_{A^{\mathrm{in}}} \otimes \mathcal{H}_{Y_i^R} , \\
T &: \bigoplus_{i\in I} \mathcal{H}_{Y_i^L} \otimes \mathcal{H}_{Y_i^R} \to \mathcal{H}_{F^{\mathrm{in}}} .
\end{aligned}$$

Now, consider the graphical representation of Eq. (7.10) as an extended circuit diagram as in Fig. 6.6. By bending those wires down that correspond to A^{in} and B^{in}, so as to re-identify the quantum nodes A and B, the graphical representation of the unitary process in Fig. 7.2a can be 'filled in' to yield the extended circuit decomposition[5] of the quantum SWITCH as shown in Fig. 7.6

[5]The way the graphical notation from Chap. 6 has been deployed here may more appropriately be called 'extended string diagrams', since it additionally allows liberally bending wires around, using 'cups and caps' (see, e.g., Ref. [24]). Typically, 'circuit diagrams' refer to diagrams, where the outputs of boxes can only be connected to the inputs of other boxes, while 'string diagrams' are the more general class, where anything can be connected to anything.

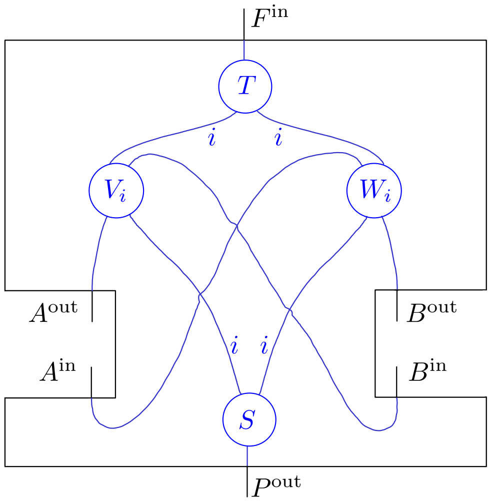


Figure 7.6: The extended circuit decomposition of the quantum SWITCH.

For the quantum SWITCH it is straightforward to see what the decomposition in Eq. (7.10) is concretely. The index i is binary and the two values, say 0 and 1, can be seen to label the corresponding subspaces of the control qubit Q. This subspace decomposition of Q induces the corresponding decomposition of P^{out}, as identified by the unitary S:

$$\mathcal{H}_{P^{\text{out}}} = \mathcal{H}_Q \otimes \mathcal{H}_S \;\cong\; (\mathcal{H}_S \otimes \mathbb{C}) \oplus (\mathbb{C} \otimes \mathcal{H}_S) =: (\mathcal{H}_{X_0^L} \otimes \mathcal{H}_{X_0^R}) \oplus (\mathcal{H}_{X_1^L} \otimes \mathcal{H}_{X_1^R}) \, .$$

The unitary V_i is the SWAP transformation on the respective systems for $i = 0$ and the identity map on A^{out} (X_1^L is trivial) in case of $i = 1$[6], and similarly for W_i just with a reversed role of 0 and 1. Hence, while the causal structure of the quantum SWITCH is cyclic, each of the summands $V_0 \otimes W_0$ and $V_1 \otimes W_1$, when seen as defining a unitary process, has an acyclic causal structure.

Note that any unitary extension σ_{ABPF} of a unitarily extendible bipartite process σ_{AB} — equivalently, any unitary process σ_{ABPF} on 4 nodes, where P is a root node and F a leaf node — necessarily satisfies the two causal constraints as in Fig. 7.5 and hence, has an extended circuit decomposition of the form as in Fig. 7.6. As we argued in Ref. [3] (and as was afterwards independently shown in Ref. [164]), it then follows from the requirement that σ_{ABPF} is a process, that for each i the unitary process defined by $V_i \otimes W_i$ (where the input and output spaces of the nodes are subspaces of the corresponding spaces of the nodes $ABPF$) has an acyclic causal structure. Any such unitary process σ_{ABPF} is thus revealed, loosely speaking, 'to

[6]The terms SWAP and identity transformations are used in the obvious sense here despite that the labels of the spaces are changing.

be' a direct sum over unitary processes with an acyclic causal structure, ignoring the unitaries S and T. This is the main idea behind the proof of Theorem 3[7] of Ref. [3], which states that all bipartite unitarily extendible processes are causally separable.

7.5.2 Looking inside the BW unitary extension of the AF process

A second example of a faithful cyclic quantum causal model involving a causally non-separable process was given in Sec. 7.4.2 in terms of the tripartite AF process $\sigma^{\mathrm{AF}}_{ABC}$. While the latter is not itself a unitary process, it is unitarily extendible and Eqs. (7.8) and (7.9) stated the BW unitary extension, denoted $\sigma^{\mathrm{BW}}_{ABCFP} = \rho^{U}_{ABCF|ABCP}$. Recalling that $\mathcal{H}_{P^{\mathrm{out}}} = \mathcal{H}_{\lambda_A} \otimes \mathcal{H}_{\lambda_B} \otimes \mathcal{H}_{\lambda_C}$, the BW extension has the causal structure as depicted in Fig. 7.4, so that the associated unitary map

$$U \ : \ \mathcal{H}_{A^{\mathrm{out}}} \otimes \mathcal{H}_{B^{\mathrm{out}}} \otimes \mathcal{H}_{C^{\mathrm{out}}} \otimes \mathcal{H}_{\lambda_A} \otimes \mathcal{H}_{\lambda_B} \otimes \mathcal{H}_{\lambda_C} \ \rightarrow \ \mathcal{H}_{A^{\mathrm{in}}} \otimes \mathcal{H}_{B^{\mathrm{in}}} \otimes \mathcal{H}_{C^{\mathrm{in}}} \otimes \mathcal{H}_{F^{\mathrm{in}}}$$

satisfies the no-influence relations as illustrated through the red dashed arrows in Fig. 7.7.

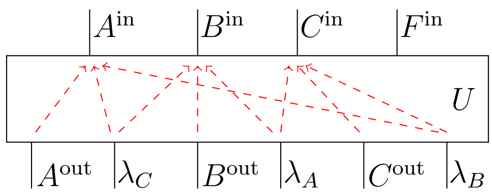
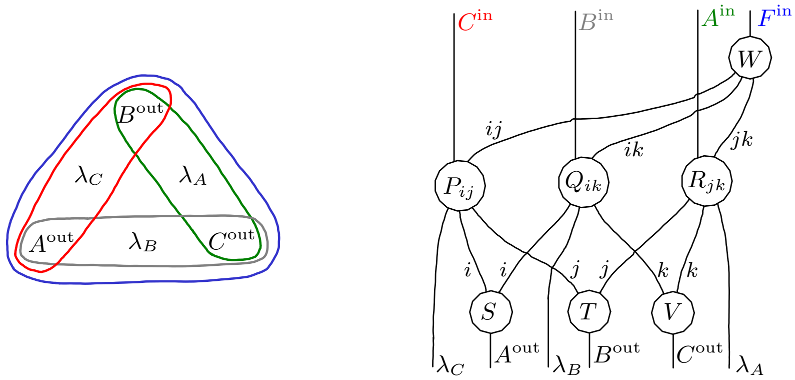


Figure 7.7: The unitary map U from Eq. (7.9) that defines the BW unitary extension of the AF process, together with, shown as red dashed arrows, the causal constraints it satisfies.

Although this particular case of a causal structure of a unitary of type $(6, 4)$ was not treated in Sec. 6.6, observe that it is similar to that in Fig. 6.21a of Thm. 6.6, except for the additional systems λ_A, λ_B and λ_C. This can be seen most easily if representing the causal structure of U as in Fig. 7.8a using the hypergraph notation of Chap. 6. The latter representation does not express anything Fig. 7.7 did not already express, but it emphasises the overlap structure between the parental sets and thereby makes evident that a proof analogous to that of Thm. 6.6 in App. B.4 straightforwardly yields the following result.

[7]This result is due to O. Oreshkov and therefore not presented in detail with a proof in this thesis.

Theorem 7.2 *Given a unitary transformation* $U : \mathcal{H}_{A^{out}} \otimes \mathcal{H}_{B^{out}} \otimes \mathcal{H}_{C^{out}} \otimes \mathcal{H}_{\lambda_A} \otimes \mathcal{H}_{\lambda_B} \otimes \mathcal{H}_{\lambda_C} \to \mathcal{H}_{A^{in}} \otimes \mathcal{H}_{B^{in}} \otimes \mathcal{H}_{C^{in}} \otimes \mathcal{H}_{F^{in}}$*, if the causal structure of* U *is as in Fig. 7.8a, then* U *has a causally faithful extended circuit diagram as shown in Fig. 7.8b.*



(a) (b)

Figure 7.8

Proof. Analogous to the proof of Thm. 6.6 in App. B.4. □

For the sake of completeness, the decomposition from Fig. 7.8b written out algebraically, reads:

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

for (families of) unitary maps

$$S : \ \mathcal{H}_{A^{\text{out}}} \ \to \ \bigoplus_i \mathcal{H}_{X_i^L} \otimes \mathcal{H}_{X_i^R}, \qquad P_{ij} : \ \mathcal{H}_{\lambda_C} \otimes \mathcal{H}_{X_i^L} \otimes \mathcal{H}_{Y_j^L} \ \to \ \mathcal{H}_{C^{\text{in}}} \otimes \mathcal{H}_{G_{ij}^{(1)}},$$

$$T : \ \mathcal{H}_{B^{\text{out}}} \ \to \ \bigoplus_j \mathcal{H}_{Y_j^L} \otimes \mathcal{H}_{Y_j^R}, \qquad Q_{ik} : \ \mathcal{H}_{X_i^R} \otimes \mathcal{H}_{\lambda_B} \otimes \mathcal{H}_{Z_k^L} \ \to \ \mathcal{H}_{B^{\text{in}}} \otimes \mathcal{H}_{G_{ik}^{(2)}},$$

$$V : \ \mathcal{H}_{C^{\text{out}}} \ \to \ \bigoplus_k \mathcal{H}_{Z_k^L} \otimes \mathcal{H}_{Z_k^R}, \qquad R_{jk} : \ \mathcal{H}_{Y_j^R} \otimes \mathcal{H}_{Z_k^R} \otimes \mathcal{H}_{\lambda_A} \ \to \ \mathcal{H}_{A^{\text{in}}} \otimes \mathcal{H}_{G_{jk}^{(3)}},$$

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

In the same fashion as above for the quantum SWITCH, now considering Fig. 7.8b, bending those wires down that correspond to A^{in}, B^{in} and C^{in} to re-identify the nodes A, B and C (and swapping some wires for better readability), yields the extended circuit decomposition of the BW unitary extension as shown in Fig. 7.9 — a fine-grained compositional structure of the process that makes clear what the pathways of causal influence are. It is again not difficult to see what the data in Fig. 7.9 is for the concrete case of the BW unitary extension. All three indices i, j and k are binary and each 'indexed space', i.e. each element of the family of Hilbert spaces associated with an indexed wire, is a trivial Hilbert space. For any fixed tuple (i,j,k), the unitary $P_{ij} \otimes Q_{ik} \otimes R_{jk}$ is of the type $\mathcal{H}_{\lambda_C} \otimes \mathcal{H}_{\lambda_B} \otimes \mathcal{H}_{\lambda_A} \to \mathcal{H}_{C^{\text{in}}} \otimes \mathcal{H}_{B^{\text{in}}} \otimes \mathcal{H}_{A^{\text{in}}}$, where all spaces are qubits and all trivial spaces in the domain and codomain have been suppressed. The unitary $P_{ij} : \mathcal{H}_{\lambda_C} \to \mathcal{H}_{C^{\text{in}}}$ maps $|\lambda_C\rangle \mapsto |\lambda_C \oplus (\neg i \wedge j)\rangle$, i.e. P_{ij} is the identity or the NOT gate depending on the values of i and j. The unitaries Q_{ik} and R_{jk} can similarly be identified through comparison with Eq. (7.9). Thus, the BW unitary extension can be seen as a direct sum over unitary processes each of which has an acyclic causal structure.

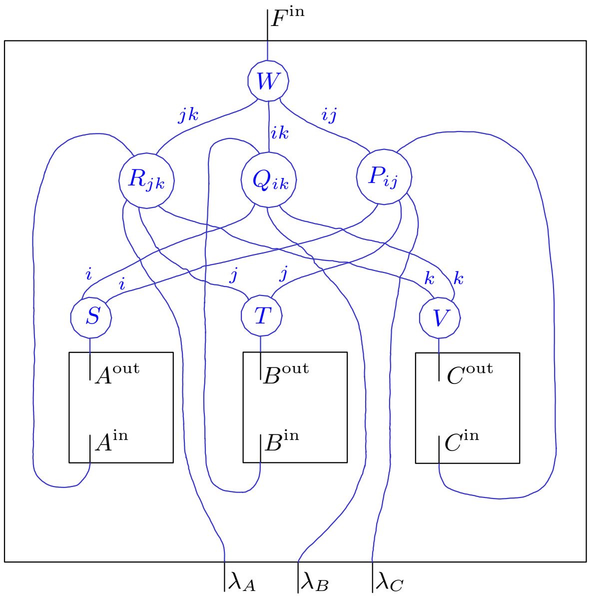


Figure 7.9: Extended circuit decomposition of the BW unitary extension of the AF process.

Note that actually any unitary process with a causal structure as in Fig. 7.4 has a decomposition of the form as in Fig. 7.9. Naturally, the question now is whether a similarly insightful decomposition exists for any unitary extension of a tripartite process, and maybe even a 'direct sum over acyclic processes' type of statement can be made, analogously to the conclusion in Sec. 7.5.1 concerning any unitary extension of a bipartite process. Suppose $\sigma_{ABCPF} = \rho^U_{ABCF|ABCP}$ is a unitary process with root node P and leaf node F, then the only causal constraints that are entailed by virtue of σ_{ABCPF} being a process are that $X^{\text{out}} \not\twoheadrightarrow X^{\text{in}}$ for all $X = A, B, C$, that is, the causal structure of the unitary map U is as in Fig. 7.10 (up to possibly further causal constraints in specific cases). However, the latter causal structure is the same as the one in Fig. 6.32, which is one for which the derivation of a causally faithful extended circuit decomposition was left as an open problem. At the time of writing, it is therefore not known yet whether the unitary extension of a tripartite process always has a decomposition as a 'direct sum over acyclic processes'.

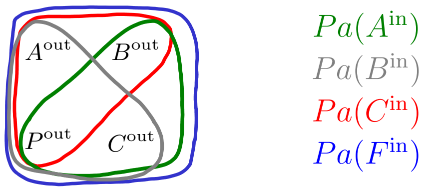


Figure 7.10: The causal structure defined by the minimum set of causal constraints of the unitary extension of a tripartite process.

7.6 Cyclicity and classical processes

7.6.1 Cyclic classical split-node causal models

The fact that there exist classical processes that are not compatible with any causal order of its classical split nodes (see Sec. 7.1.2) provides motivation to also spell out the special case of the generalised framework of quantum causal models from Def. 7.1, where the process is, in the sense of $I_{\sigma\to\kappa}$ and $I_{\kappa\to\sigma}$, classical. This gives the following generalisation of the classical split-node causal models from Def. 5.6 to cyclic causal structures.

Definition 7.5 (Classical split-node causal model): *A* Classical split-node causal model *(CSM) is given by:*

(1) *a causal structure represented by a directed graph G with vertices corresponding to classical split-nodes $X_1, ..., X_n$,*

(2) *for each X_i, a classical channel $P(X_i^{in}|Pa(X_i)^{out})$, where $Pa(X_i)$ denotes the set of parents of X_i according to G, such that $\kappa_{X_1 \cdots X_n} = \prod_i P(X_i^{in}|Pa(X_i)^{out})$ is a process operator over $X_1, ..., X_n$.*

Similarly generalising Def. 5.7, for a classical process $\kappa_{X_1 \ldots X_n}$ to be *Markov for a directed graph G* with classical split nodes $X_1, \ldots, X_n$ as its vertices, has the obvious meaning.

Note that the formal 1-to-1 correspondence in the acyclic case between classical split-node causal models and conventional classical causal models, discussed in detail in Sec. 5.3, does not extend to general directed graphs. Cyclic directed graphs have been studied and used in the context of classical causal models (see, e.g., Refs. [165–168]), but there, directed cycles are taken to represent classical feedback loops and do not exhaust the generality of classical processes including those that are incompatible with any causal order. Studying the precise relationship between the usage of cyclic directed graphs in the 'classical causal modeling literature' and the above Def. 7.5 is left for future work.

Note that in Sec. 5.3 classical split-node causal models were introduced primarily to elucidate the relation between quantum and classical causal models and to obtain the results in Secs. 5.5 and 5.6. In contrast, here the motivation is essentially the same as for the quantum case, namely, to use a causal model perspective to study the 'exotic' processes in the formalism.

7.6.2 A classical version of the conjecture

Chapter 5 did not present an explicit classical analogue of the equivalence between Markovianity and compatibility with a DAG. This was omitted because of the primarily pedagogical purpose of classical split-node causal models in that chapter and because there is little insight to be gained in merely lifting the ideas from Sec. 3.1.2 on classical causal models from underlying determinism to a formulation in terms of classical processes. This is different in the context of cyclic CSMs and the following will briefly spell out classical analogues of the concepts in Sec. 7.3.

First of all, in keeping with the spirit from Sec. 3.1.2, i.e. causal relations as relations of dependence between variables in an underlying deterministic description, causal relations pertain to deterministic processes, leading to the following classical analogue of causal structure of a unitary process.

Definition 7.6 (Causal structure of a deterministic classical process): *Given a deterministic process $\kappa^f_{X_1...X_n}$, the* causal structure *of the process is the directed graph with vertices $X_1, ..., X_n$ and an arrow $X_i \rightarrow X_j$, whenever X_j^{in} depends on X_i^{out} through the function f.*

Observe the following (proof straightforward and omitted).

Proposition 7.2 *Every deterministic classical process is Markov for its causal structure.*

Thus, just as is the case with any unitary process, any deterministic process together with its causal structure constitutes a faithful CSM.

In order to make precise the relation between generic classical processes and causal structure, we now choose to insist on reversibility for closer analogy with the quantum case in Defs. 7.3 and 7.4.

Definition 7.7 (Reversible extendibility): *A process* $\kappa_{X_1...X_n}$ *is* reversibly extendible *if and only if there exists a reversible deterministic process* $\kappa^f_{X_1\cdots X_n F\lambda}$ *with an additional leaf node* F *and root node* λ*, such that* $\kappa_{X_1\cdots X_n} = \sum_{F^{in},\lambda^{out}}[\kappa^f_{X_1\cdots X_n F\lambda} P(\lambda^{out})]$ *for some probability distribution* $P(\lambda^{out})$*.*

Definition 7.8 (Compatibility with a directed graph): *A process* $\kappa_{X_1\cdots X_n}$ *is* compatible *with a directed graph* G *with nodes* $X_1, ..., X_n$*, if and only if* $\kappa_{X_1\cdots X_n}$ *is reversibly extendible to a deterministic process* $\kappa^f_{X_1\cdots X_n F\lambda_1...\lambda_n}$*, with an additional leaf node* F*, root nodes* λ_i*, and a product distribution* $\prod_i P(\lambda_i^{out})$*, such that through* f*,* X_i^{in} *depends neither on* λ_j^{out} *for* $j \neq i$ *nor on* X_j^{out} *for* $X_j \notin Pa(X_i)$ *(with* $Pa(X_i)$ *referring to* G*).*

The choice of insisting on reversibility of the asserted deterministic process, may also seem slightly more natural from the point of view of fundamental physics, but note that this really is just a matter of analogy to the quantum case, since any deterministic process can be extended to a reversible deterministic process without introducing further common causes [58][8].

The following analogue of Thm. 7.1 is straightforward due to Prop. 7.2.

Theorem 7.3 *If a classical process* $\kappa_{X_1\cdots X_n}$ *is compatible with a directed graph* G*, then it is also Markov for* G*.*

The converse direction does not seem straightforward, also in this classical case (cf. Conjecture 1), and it is stated as a conjecture.

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

Note that the relation to the quantum version, Conjecture 1, is a priori not just one of being a special case of the latter. It has not been established yet whether reversible extendibility implies unitary extendibility for a classical process when seen as a special case of a quantum process [58]. Hence, if Conjecture 2 is true, it does note immediately give the quantum conjecture on the special cases of classical prcoesses. Conversely, if Conjecture 1 holds, then Conjecture 2 is not immediately implied: if a classical process that is Markov for a given graph, admits a unitary extension (seeing it as a quantum process), which satisfies the corresponding causal

[8]The statement of this result, Theorem 2 in Ref. [58], only introduces one leaf and one root node, however, the proof in fact uses an output variable of the additional root node that has a Cartesian product structure such that it can be thought to constitute n distinct root nodes if there were n originally given nodes $X_1, ..., X_n$ and such that each new root node is a cause of at most one of the X_i.

constraints to establish quantum compatibility with the graph, it is not necessarily clear that any of the unitary extensions define a reversible deterministic classical process for the special basis fixed by the given classical process.

We close the discussion of classical processes with the following observation.

Theorem 7.4 *Given a set of classical split nodes $X_1, ..., X_n$, the set of reversibly extendible classical processes on $X_1, ..., X_n$ coincides with the deterministic polytope.*

Proof: See App. C.5. □

Thus, in case Conjecture 2 is true, it follows that all classical processes that are part of a classical split-node causal model, i.e. Markov for a directed graph, have to lie inside the deterministic polytope. A well-known example of a classical process that lies outside the deterministic polytope was found in Ref. [52] (therein denoted $\hat{E}_{ex1}$). One can easily check that this process is indeed not Markov for any directed graph[9], hence in keeping with Conjecture 2.

7.7 Quantum causal inference 2.0

Let us return to the causal inference perspective that already underlay Sec. 5.7.3. Call a process $\sigma_{A_1...A_n}$ *causally explicable* if it can be seen to arise from a (possibly cyclic) quantum causal model with process $\sigma_{A_1...A_nL}$, that has a set L of additional, latent nodes and is such that for some intervention τ_L, the original process is obtained back, $\sigma_{A_1...A_n} = \mathrm{Tr}_L\big[\sigma_{A_1...A_nL}\ \tau_L\big]$. One of the main questions then becomes which quantum processes are causally explicable at all within the presented framework.

The following does not present much substantial new insight, but is included for the sake of completeness and overview. It essentially gives a case differentiation of how a process $\sigma_{A_1...A_n}$ can stand to its induced graph G_σ (cf. Def. 5.24), presented as the sketch of a causal discovery algorithm that generalises the one from Ref. [121] and extends one from Sec. 5.7.3 to the generalised framework.

Given a process $\sigma_{A_1...A_n}$, calculate G_σ, that is, the parental sets $\{Pa(A_i)\}_{i=1}^n$ by checking the corresponding $n(n-1)$ linear constraints from Eq. (5.35) in Sec. 5.7.3. Then check whether G_σ is a DAG or not.

(1) If it is a DAG, check whether $\sigma_{A_1...A_n}$ is Markov for G_σ, i.e. check whether the marginal channels, $\rho_{A_i|Pa(A_i)}$ and $\rho_{A_j|Pa(A_j)}$ (already calculated as part of

[9]Note that Rem. 5.9 generalises to cyclic directed graphs and applies in particular to the subset of classical processes. It is therefore enough to check Markovianity for the induced direct-signalling directed graph.

finding G_σ), commute whenever $Pa(A_i) \cap Pa(A_j) \neq \emptyset$ and $i \neq j$ and if so, whether $\sigma_{A_1 \ldots A_n} = \prod_i \rho_{A_i|Pa(A_i)}$[10].

(A) If yes, return (G_σ, acyclic, Markov).

(B) If not, check whether $\sigma_{A_1 \ldots A_n}$ is a quantum comb.

(a) If a comb, return (G_σ, acyclic, not Markov, Comb).

(b) Otherwise return (G_σ, acyclic, not Markov, not Comb).

(2) If G_σ is not a DAG, check whether $\sigma_{A_1 \ldots A_n}$ is Markov for G_σ (same as in (1)).

(A) If yes, return (G_σ, cyclic, Markov).

(B) If not, return (G_σ, cyclic, not Markov).

First, note that Rem. 5.9 generalises to arbitrary directed graphs, i.e. a process $\sigma_{A_1 \ldots A_n}$ is either Markov for its induced graph G_σ and then for any directed graph which contains G_σ as a subgraph, or else, it is not Markov for any directed graph with vertices $A_1, \ldots, A_n$. Causal discovery can therefore be reduced to the search of faithful (cyclic) QCMs in the sense as explained in Sec. 5.7.3. Furthermore, note that classical processes and their explanations in terms of (cyclic) classical split-node causal models are contained in the above as special cases[11]

Now, in case of (G_σ, acyclic, Markov) or (G_σ, cyclic, Markov) the given process $\sigma_{A_1 \ldots A_n}$ already defines a faithful quantum causal model, i.e. G_σ is a candidate causal explanation of the given process. As already mentioned in Sec. 5.7.3, in case of (G_σ, acyclic, not Markov, Comb), one concludes that $\sigma_{A_1 \ldots A_n}$ is causally explicable, but that common causes are necessarily missing in the set of nodes $\{A_1, \ldots, A_n\}$.

The cases of (G_σ, acyclic, not Markov, not Comb) and (G_σ, cyclic, not Markov) are inconclusive and contain causally explicable as well as inexplicable ones — a distinction that essentially comes down to unitary extendibility. Note that Ref. [123] presented a necessary, but not sufficient condition for unitary extendibility, and an easy-to-check condition that allows to determine whether a process is unitarily extendible, is still missing. Ignoring such computational issues, in case $\sigma_{A_1 \ldots A_n}$ is not Markov, but unitarily extendible, the unitary extension defines a QCM, hence $\sigma_{A_1 \ldots A_n}$ is causally explicable and one concludes that common causes to the nodes $\{A_1, \ldots, A_n\}$ are necessarily missing. It is left for future work to study in detail

[10] Checking Markovianity thus amounts to checking at most $n(n-1)+1$ further linear constraints.

[11] The remainder of this section and the subsequent one discuss the dependence of causal inference on the validity of the quantum Conjecture 1. Also for the classical Conjecture 2 an analogous discussion can be held, but will be omitted.

when and how one can infer more about the kind of latent common causes that need to be involved, such as which subsets of $\{A_1, \ldots, A_n\}$ they affect. In case $\sigma_{A_1 \ldots A_n}$ is not unitarily extendible, then — assuming the validity of Conjecture 1 — $\sigma_{A_1 \ldots A_n}$ cannot possibly arise from a QCM, hence is not causally explicable. A discussion of what to conclude in case Conjecture 1 is false is postponed to the next section.

7.8 Discussion

This chapter answered positively the question from Sec. 7.2.1 of whether or not a framework of quantum causal models can be developed that also applies to causally nonseparable processes. It did so by extending the framework from Chap. 5 to cyclic causal structures. Now, what is gained through that extension?

As illustrated through the examples of the quantum SWITCH (Sec. 7.4.1) and the AF process (Sec. 7.4.2), the framework provides the grounds on which certain causally nonseparable processes can now be given a causal explanation — in terms of cyclic causal structure. The conceptual step thereby rendered possible is to go from seeing certain processes as having an 'indefinite causal order' to having a definite causal structure, where we only had to revise what the properties of the latter are in general. Similarly, processes that are called noncausal — a term suggesting they cannot be understood causally — turn out, at least some of them, to only defy the notion of causal (partial) order, but are very much amenable to causal analysis. The new notions of 'causal' and 'noncausal', as it were, are whether a process $\sigma_{A_1 \ldots A_n}$ is *causally explicable* or not within the framework (see previous section for causal explicability).

The main insight may thus be seen to be that the notion of cyclic causal structure can be given rigorous meaning within the new framework and the main, albeit tentative proposal to take that notion seriously.

Cyclicity, causal (non)separability and extended circuit decompositions

Section 7.2.2 observed the difference between, on the one hand, the bipartite cyclic directed graph in Fig. 7.1a not being a possible causal explanation[12] of any bipartite process σ_{AB} and, on the other hand, the tripartite cyclic graph in Fig. 7.1b being a possible causal explanation of some processes σ_{ABC} (namely, whenever the latter is Markov for the graph in Fig. 7.1b). It was claimed that this difference comes down to the fact that in the second case there is an additional common cause to A

[12]Restricting to faithful quantum causal models here.

and B given by C, which manifests itself in the overlap of the non-trivial action of the two commuting operators $\rho_{A|BC}$ and $\rho_{B|AC}$ from Eq. (7.4) on C^{out}, and that it is the corresponding decomposition of the operators due to Lem. 4.1, which allows to understand the 'cycle of causal influence without leading to contradictions'.

One way to substantiate this claim is provided by the results from Sec. 7.5 in terms of extended circuit decompositions. A unitary process σ_{ABCF} with leaf node F and root node C has an extended circuit decomposition such that, loosely speaking, in any one subspace there is at most signalling from A to B or vice versa [3]. Now, the marginal process from marginalising over the node F is precisely of the form as in Eq. (7.4)[13]. Similarly, the extended circuit decomposition of the BW extension of the AF process turned out to be a direct sum over unitary processes with an acyclic causal structure (see Fig. 7.9).

This is suggestive of that there might be a more general understanding to be obtained concerning the relation between causally nonseparable processes and extended circuit decompositions — it is at least conceivable that all unitary processes might turn out to be 'direct sums over unitary processes with acyclic causal structure'[14]. This provides further motivation to go beyond the thus far obtained results in Sec. 6.6 and, ultimately, to try to prove or else disprove Hypothesis 1. Together with the result from Ref. [3] that a unitary process is causally nonseparable if and only if it has a cyclic causal structure[15], there lies a potential for a substantially better understanding of causally nonseparable processes.

What if Conjecture 1 is false?

Suppose Conjecture 1 is false. How does that change the set of causally explicable processes and their status? A priori, a false Conjecture 1 leaves two conceiveable logically distinct situations. Either all processes $\sigma_{A_1 \ldots A_n}$ that are Markov, are unitarily extendible, however, they do not generally allow for a unitary extension with the appropriate causal structure so as to establish compatibility with G_σ. Alternatively, it is not even true that all processes that are Markov, also are unitarily extendible. In either case, if Conjecture 1 is false, there exist processes that satisfy the Markov condition, but where it is impossible to give that Markovianity the meaning otherwise intended by the framework.

[13]Provided Conjecture 1 holds, also the converse is true, i.e., whenever a tripartite process of the form as in Eq. (7.4) is given, then it has an extension to a unitary process which has an extended circuit decomposition essentially of the same form as in Fig. 7.6 (up to some additional local causes).

[14]I thank J. Barrett for formulating this intuition clearly for the first time.

[15]This result (Theorem 4 in Ref. [3]) is not presented in this thesis as it is largely due to my co-authors, in particular O. Oreshkov.)

Instead of abandoning the notion of cyclic quantum causal models altogether, the proposed lesson to take away in such a case would be that, beyond acyclic causal structures, the Markov condition is a misleading one and has to be abandoned. In order to explain this further, first note that also in the acyclic regime, one could have presented the framework as built on two notions: (1) the definition of a quantum causal model as a unitary process with an acyclic causal structure (2) the notion of compatibility with a DAG from Def. 5.3 as the relevant condition for when to take a particular DAG as a candidate causal explanation of a non-unitary process. What the equivalence in Thm. 5.2 achieves is just establishing a more convenient definition of a quantum causal model to work with, seeing that in so far as it is an empirical framework, one will rarely be dealing with unitary processes, but typically with non-unitary process operators estimated from experimental data. This is in fact mirroring how Pearl presents classical causal models in Ref. [9], namely, as functional models and only once the equivalence between Markovianity and compatibility[16] is established, the working definition of a causal model is a DAG G and a distribution that is Markov for G.

In keeping with the outlined spirit, in case Conjecture 1 is false, the general framework would have to be presented as: (1) the definition of a quantum causal model as a unitary process together with its causal structure and (2) the notion of compatibility with a directed graph from Def. 7.4 as the relevant condition for when to take a particular directed graph as a candidate causal explanation of a non-unitary process. Thus, in the template of an algorithm sketched in Sec. 7.7, step (2) would then be dropped, while it remains to be the case that $\sigma_{A_1 \dots A_n}$ is causally explicable if and only if is unitarily extendible, as previously, only with a changed definition of a QCM that underlies 'causal explicability'. If causal structure pertains to unitary processes, it indeed should be a tautology that causal explicability reduces to unitary extendibility.

Physicality of processes

One of the main open questions of the field, as mentioned in Sec. 7.1, concerns which processes are 'physical', that is, realisable in nature in some sense or other. In Ref. [123], unitary extendibility was originally proposed as a postulate to discern physical from unphyscial processes, that is, unitary extendibility is considered a necessary, albeit maybe not sufficient, condition for physicality.

The motivation for this proposal came primarily from observing 'reversibility' as a cherished principle in physics together with the fact that, as shown in Ref. [123],

[16]This terminology was not used by Pearl, but introduced in Ref. [4] and is useful to succinctly describe Pearl's approach.

unitary processes are precisely those, which map unitary channels to unitary channels, i.e. they are the higher-order maps that preserve purity and reversibility.

Independently from the validity of Conjecture 1, modulo the wrinkle explained just above, the unitarily extendible processes are precisely the causally explicable ones. One may see this as an independent reason for considering unitary extendibility a necessary condition for physicality, asserting that only processes that are amenable to a causal analysis can be physical.

Chapter 8

Conclusions

8.1 Summary

This section summarises the main results presented in this thesis. For more in-depth discussions see in particular Secs. 5.2.4, 5.7 6.9 and 7.8.

Recall from the introduction in Chapter 1 the two steps (1) and (2), that were formulated as an approach to provide a conceptual grounding for a quantum causal model framework. Chapter. 4 took step (1): in Def. 4.6 the *direct cause relation* was defined as the relation between quantum nodes C and E relative to a unitary process $\sigma_{CE...} = \rho^U_{CE...|CE...}$ with the causal connection given by influence from C^{out} to E^{in} in the associated unitary map U. Any unitary process then has a *causal structure* (Def. 4.7) given by the set of all direct cause relations, representable as a directed graph. Special cases of unitary processes are ordinary unitary channels $\rho^U_{C_1...C_k|B_1...B_n}$, where $B_1, \dots, B_n$ are root nodes and $C_1, \dots, C_k$ are leaf nodes, as well as broken unitary circuits as described in Sec. 5.2.2.

The main idea is that there always is an underlying unitary process, while the generic object as a description of the behaviour of a set of quantum nodes is a non-unitary process. What *quantum causal models* are supposed to formalise is how analysing possible causal explanations in the latter case works. As far as acyclic causal structures are concerned, Chapter 5 studied the framework of quantum causal models as defined in Def. 5.1, originally proposed by Allen *et al.* in Ref. [4]. Section 5.2.3 took step (2) from our 'scheme' and established this framework as the one that captures giving causal explanations in accordance with the definitions from Chapter. 4: Theorem 5.2 finds *equivalence* between compatibility of a process $\sigma_{A_1...A_n}$ with a DAG G with vertices $A_1, \dots, A_n$ and Markovianity for G (see Defs. 5.3 and 5.2, respectively).

Section 5.3 gave a detailed analysis of how quantum and classical causal models relate to each other, the exposition of which made use of the 'intermediate kind', classical split-node causal models. Section 5.4 presented various notions of independence for classical processes and quantum processes that generalise those of unconditional and conditional independence for classical probability distributions. All discussed notions can be seen as special cases of *quantum relative independence* from Def. 5.15. See Props. 5.6 and 5.3 for corresponding operational statements for quantum and classical processes, respectively. Section 5.5 proved that *d-separation* is sound and complete for quantum relative independence. Section 5.6 presented quantum generalisations of all *three rules of the classical do-calculus*, together with operational statements implied by (equivalent to) the corresponding consequent for quantum (classical) processes. See Sec. 5.6.4 for an overview.

Chapter 6 had two aspects: first, the (algebraic) derivation of decompositions of unitary maps implied by their causal structure in terms of sequential, tensor product and direct sum compositions of unitary maps, and, second, the graphical representation of such decompositions, which relied on the introduction of *extended circuit diagrams* as a new kind of diagram. Section 6.6 presented *causally faithful* extended circuit decompositions for all unitary maps with arbitrary number of input systems if at most three output systems and with arbitrary number of output systems if at most three input systems, as well as for some unitary maps with 4 input and 4 output systems. This allows an understanding of the causal structure of unitary maps in compositional terms, where this was previously not possible.

Chapter 7 introduced a generalised framework of quantum causal models (see Def. 7.1), where the causal structure is allowed to contain directed cycles, representable by a directed graph, rather than a DAG. The proposal is that the novel *cyclic quantum causal models* may help shed light on causally nonseparable processes (see Sec. 7.1.1) and indeed, Sec. 7.4 showed the quantum SWITCH and a well-known process due to Araújo and Feix to be examples of cyclic quantum causal models. Section 7.5 showed how the results on extended circuit decompositions from Chapter 6 can provide fine-grained and insightful decompositions of causally nonseparable processes. Section 7.7 summarised what the immediate observations on quantum causal inference are, both for acyclic and cyclic causal structures, and sketched a quantum causal discovery algorithm.

As was claimed in Chapter 4, all results essentially come down to and are facilitated by two things: Theorem 4.1, the factorisation of the CJ operator of a unitary channel into commuting factors according to its causal structure, together with Lem. 4.1 that relates the commutation relations to decompositions of the underlying Hilbert spaces. It was the factorisation property from Thm. 4.1 that allowed us to see that the causal structure of a unitary transformation is a DAG at all (see Sec. 4.1). That same factorisation also is what the quantum Markov condition is understood to reflect — it comes from the underlying unitary process and is only lost if one marginalises over common causes. It is the pairwise commutation relations in light of Lem. 4.1 that enables the nontrivial part of the proof of Thm. 5.2, the proofs related to operational statements in Secs. 5.4 and 5.6, and, above all, that yields the decompositions discovered in Chapter 6, manifesting a tight relation between causal structure and direct sum structures. This highlights how the whole thesis can, also from a technical point of view, be seen as the exploration of quantum causal structure as defined in the foundational Chapter 4.

8.2 Outlook

A detailed discussion of the open questions can be found within the respective chapters. The following only briefly mentions again what could be considered to be the most important directions for future work.

Concerning the framework of acyclic quantum causal models, as covered in Chap. 5, a focus should lie on applications and practical problems. This may include extending the causal discovery algorithm so that it reveals more details about the nature of latent common causes in case of non-Markovianity of a given process σ for its induced graph G_σ (see Sec. 5.7.3). It may also include formulating a more practically relevant kind of causal discovery problem, where the given data is not a (full) process operator, as well as exploring whether there is a problem for which the generalised do-calculus rules are useful. Eventually, it would be interesting to ask whether the framework has anything to say about the existence of a meaningful notion of counterfactual relations in a quantum context.

Concerning extended circuit decompositions, studied in Chapter 6, the main open question of course is whether Hypothesis 1 is true or false. Knowing causally faithful extended circuit decompositions has already proven insightful for the structure of causally nonseparable processes in Sec. 7.5 and might quite generally prove useful for applications in quantum information theory. Hence, making progress with further causal structures, which were left open in Sec. 6.6, and, ultimately, proving or disproving the hypothesis would be valuable. Extended circuit diagrams were introduced informally in Sec. 6.4 and their formalisation as a graphical language with precise syntax and semantics should also be pursued.

Concerning cyclic causal structures, as discussed in Chapter 7, one main open problem is proving the validity or otherwise of Conjecture 1. See Sec. 7.8 for a discussion of what the consequence in either case is. Generally, it is important to further explore the framework and to consolidate the conceptual meaning of cyclic causal structure. This may well open doors, especially in combination with the techniques from Chap. 6, into a better understanding of causally nonseparable processes and even into the realisability of such processes (see Sec. 7.8). The relation to classical causal models with its use of cyclic graphs to represent feedback loops should also be studied and understood precisely.

Finally, one should explore to what extent the basic definitions of causal relations and causal structure, as well as that of quantum causal models extend to infinite dimensional Hilbert spaces.

8.3 Reflections

This section concludes the thesis with a few reflections and questions.

Quantum vs. classical causal explanations

One can present the relation between quantum causal models and classical causal models as one that focuses on similarities as much as on differences. Similarity consists in the initial motivation to make causal reasoning precise and scientific. Similarity also consists in a largely analogous form that the definitions of the main concepts themselves take, as well as the overall presentation of the material in Chap. 5 and Chap. 3. However, there also are crucial differences. One that was emphasised throughout the thesis is the conceptual and empirical difference between a probability distribution (suppose estimated from observational data) and a quantum process (or a classical process for that matter). Another difference is slightly more subtle and concerns both what the explanandum is, that is, what begs the question, and the explanans, namely where our initial intuition and confidence rests when it comes to the criterion for a successful causal explanation. This is most clearly pinned down in the simplest of cases, the common cause scenario, which was discussed in great detail in Ref. [4], as summarised in Sec. 3.2.5.1, and is recapitulated below to reflect on the difference.

Classically, the fact in need of explanation is the correlation between two variables, say Y and Z, and what Reichenbach's common cause principle demands (in case neither is a cause of the other) really is quite intuitive: once one holds the complete common cause variable X fixed, the correlation between Y and Z disappears, because there is nothing else anymore that 'ties them together'. Now, one can derive the principle as a theorem based on a functional model view, that is, by assuming an underlying determinism (see Sec. 3.1.2 and Ref. [4]). If one had doubts about the universal validity of the principle in the first place and independently from quantum physics (see Ref. [7] for an overview of challenges to the principle), then the deterministic perspective may or may not add much credence to the principle. However, for all practical purposes, the principle's important role in scientific reasoning seems to remain in any case.

Quantumly, the situation is different. The closest analogue considers a given state ρ_{BC} that is *not* of a product form, i.e. $\rho_{BC} \neq \rho_B \otimes \rho_C$, and sees that as a fact in need of causal explanation. According to the quantum common cause principle (Principle 2) if system A is a complete common cause, then for the channel $\rho_{BC|A}$ that gives rise to the state ρ_{BC} via $\rho_{BC} = \overline{\mathrm{Tr}}_A[\rho_{BC|A}\ \rho_A]$ for some state ρ_A, it holds that $\rho_{BC|A} = \rho_{B|A}\ \rho_{C|A}$. Now, even given one knows that $\rho_{BC|A} = \rho_{B|A}\ \rho_{C|A}$ holds and that ρ_A was successfully prepared at the common cause A, nothing changes the form of the state ρ_{BC} and that for at least some measurements at B and C the outcomes will be correlated conditional on the preparation of ρ_A. In that respect the situation is no different than if ρ_{BC} was described as arising from a channel for which $\rho_{BC|A'} \neq \rho_{B|A'}\ \rho_{C|A'}$. So, the intuition for the principle does *not* come from an intuitive understanding of the constraint it imposes. Instead, the credence in the principle stems entirely from the definition of causal relations and causal structure in Chap. 4: as discussed in Sec. 3.2.5.1, only if $\rho_{BC|A} = \rho_{B|A}\ \rho_{C|A}$ holds, can one justifiably claim A is a complete common cause based on those definitions [4].

For the general case of an arbitrary causal structure given by some DAG, it is again the definition of causal relations from Chap. 4, from which credence in the general causal principle (Principle 3) comes. This was established by the first main results in Sec. 5.2.

Who or what carves up the universe?

It is worth emphasising again that the causal structure of a unitary transformation $U : \mathcal{H}_{A_1} \otimes \ldots \otimes \mathcal{H}_{A_n} \to \mathcal{H}_{B_1} \otimes \ldots \otimes \mathcal{H}_{B_k}$ is only well-defined given that the specification of the map comes with a fixed tensor product structure for domain and codomain, with the subsystems taking the role of causal relata. A coarsened or a more fine-grained factorisation, or a completely different factorisation altogether, obviously leads to a different causal structure. Similarly, the causal structure of a unitary process $\sigma_{A_1 \ldots A_n}$ is only defined relative to the given set of quantum nodes. In particular, whether the causal relation between nodes A_i and A_j is a direct or indirect one depends on the overall set of nodes, just as it depends on the choice of variables for classical causal models.

This can be regarded an instance of ‘a feature, not a bug’ — causal reasoning only makes sense relative to a set of considered relata. However, the story about where this set comes from is not part of the framework of causal models that formalises causal reasoning about any *given* set. In contexts where classical causal models are useful, very different purposes or theories may tell us what the relevant relata are — clearly, a judge and a biochemist will generally be looking for quite different sorts of things as relata (also see discussion on difference between causes and background conditons in philosophy of causation [94]). Similarly in the quantum case, whatever it is that fixes a choice of systems or nodes also influences what status one may attribute to them. In a realist view, the factorisation of a Hilbert space that determines the causal analysis may be the ‘preferred’ one that corresponds to the systems out there. In an operationalist view, the kinds of nodes that have meaning are those that are defined by what an agent can do in a lab. The concept of a quantum node is abstract and generic, and *intended* to fit any approach, the hope being that the structure of causal reasoning is independent from one’s choice and correctly formalised by the framework of quantum causal models.

That said, it is an important task to develop a clear understanding of the dependence of the presented work, in particular the definition of causal relations and causal structure in Chap. 4, on assuming the standpoint of a particular interpretation of the quantum formalism. Do the definitions fix where in the ontic-epistemic divide of the quantum formalism causal relations reside? Can the definitions be sound from the perspective of, for instance, a relational interpretation [169, 170] or does it become a nonsensical undertaking from the beginning? Would it be naive to even consider the possibility that, conversely, a formalisation of causal reasoning, for instance as undertaken in this thesis, could provide new angles on old debates?

Symmetric causal relations?

The introduction started the motivation for this work by asking what to make of the progress due to classical causal models from the perspective of physics. A first reaction right then could have been that there should be no place at all in fundamental physics for caring about causal relations, as echoed in Russell’s famous line “The law of causality, I believe, like much that passes muster among philosophers, is a relic of a bygone age, surviving, like the monarchy, only because it is erroneously supposed to do no harm.” [171]. Not only do physics textbooks (mostly) not need the concept of causation to present our best candidates for fundamental theories, but also (almost) all equations of motion are time-reversal invariant. Deeming the arrow of time a non-fundamental phenomenon, similarly deprives causation of a fundamental status — so at least the claim, assuming that the causal arrow must hinge on the temporal one.

While this thesis has nothing to say about the origin of the arrow of time, it seems there are at least two reactions to such criticism that might let one see value in pursuing quantum causal models. First, as a matter of fact, the way the quantum formalism is employed and used to describe experiments in the lab, or in the development of technology, is in a time asymmetric way. So, even if deemed non-fundamental, causal reasoning may still be a crucial part of scientific practice, in particular when it involves quantum physics.

Second, it is a priori not the case that a non-fundamental status of the perceived temporal asymmetry necessarily leads to a debunking of causation in physics. One may indeed contemplate the possibility of causation being more fundamental than an arrow of time. This could be in the sense of reducing the temporal arrow to a causal arrow. However, this could also be in the sense of asserting the causal connection to constitute a symmetric relation, while the directionality, with which we usually regard the causal relation as asymmetric — as one between cause and effect — reduces to the same temporal arrow as ever, that is, insofar as there is a causal *arrow* it is the same as the temporal arrow, but this is not the essence of the causational link. While any solid argument for any possible assertion of how causal and temporal relations stand to each other is far beyond the scope of this thesis, note that Thm. 6.4 in fact establishes a sense of reversibility of the causal structure of a unitary transformation. Hence, could this fact potentially be interpreted as supporting the idea that causal structure is a set of symmetric relations amounting to which systems are causally connected to each other — no matter which 'way round one looks at' the unitary transformation?

Such and other difficult questions rely on having defined causal relations, for one otherwise does not know what one is debunking or arguing for. A small contribution towards at least one possible way of doing that, is what this thesis hopes to have done.

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Appendix A

Proofs and supplementary material Chapter 5

A.1 Useful tools I

Lemma 4.1, which will play a central role in many of the following proofs, stated how the commutation of the CJ operators of two channels, $\rho_{A|CD}$ and $\rho_{B|DE}$, implies a decomposition of $\mathcal{H}_D$, on which the non-trivial actions of both operators overlap, namely $\mathcal{H}_D = \bigoplus_i \mathcal{H}_{D_i^L} \otimes \mathcal{H}_{D_i^R}$, such that $\rho_{A|CD}\ \rho_{B|DE} = \bigoplus_i \rho_{A|CD_i^L} \otimes \rho_{B|D_i^R E}$. The below lemma describes a 'nested' such decomposition and will be useful momentarily.

Lemma A.1 *Suppose the CJ operators of three channels of the form $\rho_{A|CD}$, $\rho_{B|DEF}$ and $\rho_{H|DEG}$ commute pairwise. Then there exists a 'nested' decomposition of the DE Hilbert space into orthogonal subspaces of the form*

$$\begin{aligned}
\mathcal{H}_D \otimes \mathcal{H}_E &= \Big(\bigoplus_i \mathcal{H}_{D_i^L} \otimes \mathcal{H}_{D_i^R}\Big) \otimes \mathcal{H}_E \\
&= \bigoplus_i \mathcal{H}_{D_i^L} \otimes \Big(\bigoplus_{j_i} \mathcal{H}_{(D_i^R E)_{j_i}^L} \otimes \mathcal{H}_{(D_i^R E)_{j_i}^R}\Big) \qquad \text{(A.1)}
\end{aligned}$$

such that the given channels are block diagonal with respect to this decomposition in the following way:

$$\rho_{A|CD} = \sum_i \rho_{A|CD_i^L} \otimes \mathbb{1}_{(D_i^R)^*} , \qquad \text{(A.2)}$$

$$\rho_{B|DEF} = \sum_{i,j_i} \mathbb{1}_{(D_i^L)^*} \otimes \rho_{B|(D_i^R E)_{j_i}^L F} \otimes \mathbb{1}_{((D_i^R E)_{j_i}^R)^*} , \qquad \text{(A.3)}$$

$$\rho_{H|DEG} = \sum_{i,j_i} \mathbb{1}_{(D_i^L)^*} \otimes \mathbb{1}_{((D_i^R E)_{j_i}^L)^*} \otimes \rho_{H|(D_i^R E)_{j_i}^R G} . \qquad \text{(A.4)}$$

Proof. The proof is a mere iterative application of Lem. 4.1. We will not give a full proof here since Lem. 6.3, proven in App. B.5, is the 'same' statement only stated more carefully and does not suppress the unitary maps which define the 'decompositions'. ☐

Remark A.1 *An important special case of commuting CJ operators of channels is when the overall channel is a unitary one. Suppose* $\rho^U_{AB|CDE} = \rho_{A|CD}\rho_{B|DE}$ *represents a unitary channel. Lem. 4.1 implies a block-diagonal form* $\rho^U_{AB|CDE} = \bigoplus_i \rho_{A|CD^L_i} \otimes \rho_{B|D^R_i E}$ *relative to a decomposition of* $\mathcal{H}_D$ *into orthogonal subspaces. However the unitary of* U *means* $\rho^U_{AB|CDE}$ *is a rank-1 operator and cannot have contributions from more than one subspace. Hence, there has to exist a global factorisation* $\mathcal{H}_D = \mathcal{H}_{D^L} \otimes \mathcal{H}_{D^R}$ *such that* $\rho^U_{AB|CDE} = \rho_{A|CD^L} \otimes \rho_{B|D^R E}$. *An analogous statement holds for the nested decomposition in Lem. A.1.*

A.2 Proof of Theorem 5.1

Let G be a DAG with nodes $A_1, \ldots, A_n$, labelled such that the total order $A_1 < \cdots < A_n$ is compatible with the partial order defined by G. Consider a unitary process $\sigma_{A_1 \ldots A_n \lambda_1 \ldots \lambda_n F} = \rho^U_{A_1 \ldots A_n F | A_1 \ldots A_n \lambda_1 \ldots \lambda_n}$ which respects the causal constraints in Eq. 5.3 with $Pa(A_i)$ referring to the DAG G. The causal parents of A_i as defined by the unitary process thus have to be contained in $Pa(A_i) \cup \{\lambda_i\}$ and from Thm. 4.1 it then follows that

$$\rho^U_{A_1 \ldots A_n F | A_1 \ldots A_n \lambda_1 \ldots \lambda_n} = \rho_{F|A_1 \ldots A_n \lambda_1 \ldots \lambda_n} \left(\prod_{i=1}^{n} \rho_{A_i | Pa(A_i) \lambda_i} \right) . \tag{A.5}$$

Noting that all root nodes λ_i have a trivial input space, it will be convenient to write $\mathcal{H}_{\lambda_i}$ for $\mathcal{H}_{\lambda_i^{\text{out}}}$. Similarly for the leaf node F, write $\mathcal{H}_F$ for $\mathcal{H}_{F^{\text{in}}}$. The total order $A_1 < \cdots < A_n$ can be uniquely extended to the $2n+1$ nodes: $\lambda_1 < A_1 < \lambda_2 < A_2 < \ldots < \lambda_n < A_n < F$. Now consider the following data:

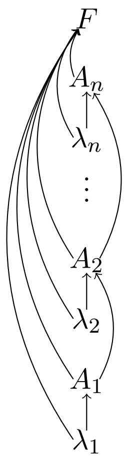


Figure A.1: DAG G'

Set A	Set B
$\rho_{F\vert\lambda_1 A_1 \ldots \lambda_n A_n}$	$\rho_{F\vert\lambda_1 A_1 \ldots \lambda_n A_n}$
$\rho_{A_n\vert Pa(A_n)\lambda_n}$	$\rho_{A_n\vert\lambda_1 A_1 \ldots \lambda_{n-1} A_{n-1} \lambda_n}$
ρ_{λ_n}	ρ_{λ_n}
$\vdots$	$\vdots$
$\rho_{A_2\vert Pa(A_2)\lambda_2}$	$\rho_{A_2\vert\lambda_1 A_1 \lambda_2}$
ρ_{λ_2}	ρ_{λ_2}
$\rho_{A_1\vert\lambda_1}$	$\rho_{A_1\vert\lambda_1}$
ρ_{λ_1}	ρ_{λ_1}

The DAG G' is obtained from drawing an arrow from λ_i to A_i for all i, drawing an arrow into F from all preceding nodes and drawing arrows between nodes A_i as given by the original DAG G. The product of channels in *Set A*, where $Pa(A_i)$ refers to the parental structure of G, is by construction Markov for G'. Focusing on the channels in *Set B*, these are obtained by padding those in Eq. A.5 with identities:

$$\rho_{A_i|\lambda_1 A_1 \ldots \lambda_{i-1} A_{i-1} \lambda_i} \;:=\; \rho_{A_i|Pa(A_i)\lambda_i} \otimes \mathbb{1}_{\overline{(Pa(A_i)\lambda_i)}} \ , \tag{A.6}$$

where $\overline{(Pa(A_i)\lambda_i)}$ denotes the relative complement of $Pa(A_i) \cup \{\lambda_i\}$ in the set $\{\lambda_1, A_1, \ldots, \lambda_{i-1}, A_{i-1}, \lambda_i\}$ and for better readability the notation in Eq. (A.6) suppresses that it is the duals of the output spaces of the nodes in $\overline{(Pa(A_i)\lambda_i)}$ that the identity operator acts on. Since the main difficulty in this proof really just is maintaining a clear notation in clunky bookkeeping, we will generally suppress the 'star' in the subscript of identity operators, letting the context make clear on which space the identity acts. It follows from the pairwise commutation of the operators defined in Eq. A.6 that

$$\left[\rho_{A_1|\lambda_1} \ , \ \rho_{A_2 \ldots A_n F|\lambda_1 A_1 \ldots \lambda_n A_n}\right] \;=\; 0 \ . \tag{A.7}$$

The unitarity of U, along with Thm. 4.1 and Rem. A.1 then imply a factorization $\mathcal{H}_{\lambda_1} = \mathcal{H}_{(\lambda_1)^L} \otimes \mathcal{H}_{(\lambda_1)^R}$ such that

$$\rho_{A_1|\lambda_1} \;=\; \rho_{A_1|(\lambda_1)^L} \otimes \mathbb{1}_{(\lambda_1)^R} \ , \tag{A.8}$$

$$\rho_{A_2 \ldots A_n F|\lambda_1 A_1 \ldots \lambda_n A_n} \;=\; \rho_{A_2 \ldots A_n F|(\lambda_1)^R A_1 \ldots \lambda_n A_n} \otimes \mathbb{1}_{(\lambda_1)^L} \ . \tag{A.9}$$

The proof now proceeds via iterative use of Lem. A.1. In order to avoid clutter in the remainder of this proof, we will furthermore often write X instead of $\mathcal{H}_X$, e.g., writing $\lambda_1 = (\lambda_1)^L \otimes (\lambda_1)^R$, instead of $\mathcal{H}_{\lambda_1} = \mathcal{H}_{(\lambda_1)^L} \otimes \mathcal{H}_{(\lambda_1)^R}$. In the second step, the fact that

$$[\rho_{A_2|\lambda_1 A_1 \lambda_2} \ , \ \rho_{A_3 \ldots A_n F|\lambda_1 A_1 \lambda_2 A_2 \ldots \lambda_n A_n}] = 0 \ , \tag{A.10}$$

along with Lem. A.1 and Rem. A.1, implies a factorization

$$(\lambda_1)^R A_1^{\text{out}} \lambda_2 \ = \ ((\lambda_1)^R A_1^{\text{out}} \lambda_2)^L \ \otimes \ ((\lambda_1)^R A_1^{\text{out}} \lambda_2)^R \ ,$$

such that

$$\begin{aligned} \rho_{A_2|\lambda_1 A_1 \lambda_2} \ &= \ \rho_{A_2|((\lambda_1)^R A_1^{\text{out}} \lambda_2)^L} \otimes \mathbb{1}_{((\lambda_1)^R A_1^{\text{out}} \lambda_2)^R} \otimes \mathbb{1}_{(\lambda_1)^L} \ , \\ \rho_{A_3 \ldots A_n F|\lambda_1 A_1 \lambda_2 A_2 \ldots \lambda_n A_n} \ &= \ \rho_{A_3 \ldots A_n F|((\lambda_1)^R A_1^{\text{out}} \lambda_2)^R A_2 \ldots \lambda_n A_n} \otimes \mathbb{1}_{((\lambda_1)^R A_1^{\text{out}} \lambda_2)^L} \otimes \mathbb{1}_{(\lambda_1)^L} \ . \end{aligned}$$

By using the short-hand notation

$$(\overleftarrow{A_i \lambda_{i+1}}) \ := \ (\cdots(((\lambda_1)^R A_1^{\text{out}} \lambda_2)^R A_2^{\text{out}} \lambda_3)^R \cdots A_i^{\text{out}} \lambda_{i+1})^R \ , \tag{A.11}$$

the iteration of the above step yields the factorization

$$\begin{aligned} \lambda_1 \otimes A_1^{\text{out}} \otimes \ldots \otimes \lambda_n \otimes A_n^{\text{out}} \ &= \ (\lambda_1)^L \otimes ((\lambda_1)^R A_1^{\text{out}} \lambda_2)^L \otimes (((\lambda_1)^R A_1^{\text{out}} \lambda_2)^R A_2^{\text{out}} \lambda_3)^L \\ &\otimes ((\overleftarrow{A_2 \lambda_3}) A_3^{\text{out}} \lambda_4)^L \ \otimes \ \ldots \ \otimes ((\overleftarrow{A_{n-2} \lambda_{n-1}}) A_{n-1}^{\text{out}} \lambda_n)^L \\ &\otimes ((\overleftarrow{A_{n-2} \lambda_{n-1}}) A_{n-1}^{\text{out}} \lambda_n)^R \ \otimes A_n^{\text{out}} \ , \end{aligned} \tag{A.12}$$

along with channels on the respective factors such that

$$\begin{aligned} \rho^U_{A_1 \ldots A_n F|A_1 \ldots A_n \lambda_1 \ldots \lambda_n} \ &= \ \rho_{A_1|(\lambda_1)^L} \ \ \rho_{A_2|((\lambda_1)^R A_1^{\text{out}} \lambda_2)^L} \\ &\rho_{A_3|((\overleftarrow{A_1 \lambda_2}) A_2^{\text{out}} \lambda_3)^L} \ \cdots \ \rho_{A_n|((\overleftarrow{A_{n-2} \lambda_{n-1}}) A_{n-1}^{\text{out}} \lambda_n)^L} \\ &\rho_{F|((\overleftarrow{A_{n-2} \lambda_{n-1}}) A_{n-1}^{\text{out}} \lambda_n)^R A_n^{\text{out}}} \ . \end{aligned} \tag{A.13}$$

Note that all operators appearing on the right hand side of Eq. A.13 act on distinct spaces. The product of the $n+1$ operators (recalling the convention of suppressing identities) is therefore identical with the tensor product of the same $n+1$ operators: $\rho_{A_1|(\lambda_1)^L} \otimes \cdots \otimes \rho_{F|((\overleftarrow{A_{n-2} \lambda_{n-1}}) \ A_{n-1}^{\text{out}} \lambda_n)^R A_n^{\text{out}}}$. Eq. A.13 then expresses that the unitary channel corresponding to U is equal to the tensor product of channels on the right hand side, each of which thus has to be a unitary channel.

Systems A'_i $(i = 1, ..., n)$, corresponding to the unbroken wires in the circuit of Fig. 5.4, are now defined using Eq. A.12 as follows:

$$
\begin{aligned}
\mathcal{H}_{A'_1} &\cong \mathcal{H}_{(\lambda_1)^R} \ , \\
\mathcal{H}_{A'_2} &\cong \mathcal{H}_{((\lambda_1)^R A_1^{\text{out}} \lambda_2)^R} \ , \\
&\vdots \\
\mathcal{H}_{A'_n} &\cong \mathcal{H}_{((\overleftarrow{A_{n-2}\lambda_{n-1}})\ A_{n-1}^{\text{out}} \lambda_n)^R} \ .
\end{aligned}
$$

Write

$$
\rho^{I_i}_{A'_i|((\overleftarrow{A_{i-2}\lambda_{i-1}})\ A_{i-1}^{\text{out}} \lambda_i)^R} \tag{A.14}
$$

for the CJ operator corresponding to a unitary map I_i between A'_i and the indicated 'right factor' – such an I_i exists by definition of the primed systems. Then define the following channels:

$$
\begin{aligned}
\rho^{U_1}_{A_1 A'_1|\lambda_1} &:= \rho_{A_1|(\lambda_1)^L} \otimes \rho^{I_1}_{A'_1|(\lambda_1)^R} \ , && \text{(A.15)} \\
\rho^{U_2}_{A_2 A'_2|A'_1 A_1 \lambda_2} &:= \rho_{A_2|(A'_1 A_1^{\text{out}} \lambda_2)^L} \otimes \rho^{I_2}_{A'_2|(A'_1 A_1^{\text{out}} \lambda_2)^R} \ , && \text{(A.16)} \\
&\vdots \\
\rho^{U_n}_{A_n A'_n|A'_{n-1} A_{n-1} \lambda_n} &:= \rho_{A_n|(A'_{n-1} A_{n-1}^{\text{out}} \lambda_n)^L} \otimes \rho^{I_n}_{A'_n|(A'_{n-1} A_{n-1}^{\text{out}} \lambda_n)^R} \ , && \text{(A.17)} \\
\rho^{U_{n+1}}_{F|A'_n A_n} &:= \rho_{F|A'_n A_n^{\text{out}}} \ , && \text{(A.18)}
\end{aligned}
$$

which are by construction unitary channels. This notation is to be understood in the obvious way: $\rho_{A_2|(A'_1 A_1^{\text{out}} \lambda_2)^L}$ is short for $\rho_{A_2|((\lambda_1)^R A_1^{\text{out}} \lambda_2)^L}$ post-composed with the unitary map I_1, and similarly for the other channels. It remains to show that marginalizing over the primed systems to obtain a broken unitary circuit of the form of that of Fig. 5.4, given by

$$
\overline{\text{Tr}}_{A'_1,...,A'_n} \left[\rho^{U_1}_{A_1 A'_1|\lambda_1} \rho^{U_2}_{A_2 A'_2|A'_1 A_1 \lambda_2} \ \cdots \ \rho^{U_n}_{A_n A'_n|A'_{n-1} A_{n-1} \lambda_n} \rho^{U_{n+1}}_{F|A'_n A_n} \right] \ , \tag{A.19}
$$

returns the unitary channel $\rho^U_{A_1 \ldots A_n F|A_1 \ldots A_n \lambda_1 \ldots \lambda_n}$ of Eq. (A.13). This is the case by construction, since

$$
\begin{aligned}
&\overline{\text{Tr}}_{A'_1} \left[\rho_{A_2|(A'_1 A_1^{\text{out}} \lambda_2)^L} \rho^{I_2}_{A'_2|(A'_1 A_1^{\text{out}} \lambda_2)^R} \rho^{I_1}_{A'_1|(\lambda_1)^R} \right] \\
&\quad = \text{Tr}_{A'_1 A'^*_1} \left[\tau^{\text{id}}_{A'_1} \rho_{A_2|(A'_1 A_1^{\text{out}} \lambda_2)^L} \rho^{I_2}_{A'_2|(A'_1 A_1^{\text{out}} \lambda_2)^R} \rho^{I_1}_{A'_1|(\lambda_1)^R} \right] \\
&\quad = \rho_{A_2|((\lambda_1)^R A_1^{\text{out}} \lambda_2)^L} \rho^{I_2}_{A'_2|((\lambda_1)^R A_1^{\text{out}} \lambda_2)^R} \ ,
\end{aligned} \tag{A.20}
$$

and similarly for A'_i, $i = 2, \ldots, n$. □

A.3 Proof of Lemma 5.1

Suppose $\rho_{B|A}$ and $\rho_{C|A}$ represent reduced unitary channels and satisfy $[\rho_{B|A}\ ,\ \rho_{C|A}] = 0$. That $\rho_{B|A}$ is a reduced unitary channel by definition means that there exists a unitary channel $\rho^V_{BF|A}$ such that $\mathrm{Tr}_F[\rho^V_{BF|A}] = \rho_{B|A}$. By Thm. 3.4, $\rho^V_{BF|A} = \rho_{B|A}\rho_{F|A}$, hence by Remark A.1 there is a global factorization $A = A^L_b \otimes A^R_b$, with respect to which $\rho^V_{BF|A} = \rho_{B|A^L_b} \otimes \rho_{F|A^R_b}$. Similarly, there exists a unitary channel $\rho^W_{CG|A}$ such that $\mathrm{Tr}_G[\rho^W_{CG|A}] = \rho_{C|A}$ and a factorization $A = A^L_c \otimes A^R_c$ such that $\rho^W_{CG|A} = \rho_{G|A^L_c} \otimes \rho_{C|A^R_c}$.

A priori, the relation between the factorizations $A^L_b \otimes A^R_b$ and $A^L_c \otimes A^R_c$ is unknown. However, by assumption it is also true that $[\rho_{B|A}, \rho_{C|A}] = 0$. The operators $\rho_{B|A^L_b}$, $\rho_{F|A^R_b}$, $\rho_{G|A^L_c}$ and $\rho_{C|A^R_c}$ all have to represent unitary channels (for dimensional reasons and due to the purity of the operators), hence, up to normalization, can be seen as maximally entangled states. It is then straightforward to check that due to the commutation of $\rho_{B|A^L_b}$ with $\rho_{C|A^R_c}$, the operator $\rho_{C|A^R_c}$ acts trivially on A^L_b, and conversely that the operator $\rho_{B|A^L_b}$ acts trivially on A^R_c. Therefore, there exists a factorization $A = A^L_b \otimes A' \otimes A^R_c$ such that $\rho_{BC|A} = \rho_{B|A^L_b} \otimes \mathbb{1}_{(A')^*} \otimes \rho_{C|A^R_c}$. This establishes the claim. □

A.4 Useful tools II

This section presents a definition and a lemma which are purely concerned with DAGs and capture the d-separation relation of a DAG in a way that will be useful in many of the subsequent proofs.

Definition A.1 (Relation SR on the nodes of a DAG): *Let G be a DAG, with a set of nodes V. Let Y, Z and W denote arbitrary disjoint subsets of V, with $R := V \setminus (Y \cup Z \cup W)$. The 3-place relation $SR(Y, Z; W)$ holds if and only if there exist partitions of W and R*

$$R = R_Y \cup R_Z \cup R^c, \quad \text{(A.21)}$$

$$W = W_Y \cup W_Z \quad \text{(A.22)}$$

such that: if A is any of Y, Z, R_Y, R_Z or R^c, and B is any of W_Y, W_Z, Y, Z, R_Y, R_Z or R^c, then the absence of an arrow $A \to B$ in Fig. A.2 implies that for any $a \in A, b \in B$, there is no arrow in G from a to b. (NB Nodes in W_Y and W_Z can have children in any other set, but these arrows are suppressed in Fig. A.2 for better visibility.)

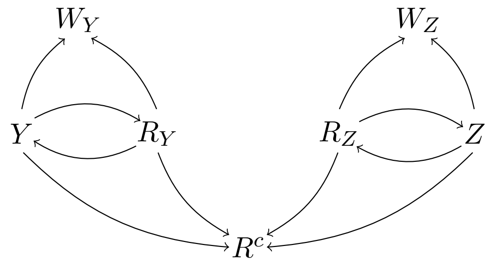


Figure A.2

Lemma A.2 *Let G be a DAG, with a set of vertices V, and let Y,Z and W be disjoint subsets of V. If $(Y \perp\!\!\!\perp Z|W)_G$, then $SR(Y, Z; W)$.*

Proof. As observed in Section 5.5 (see Refs. [96, 129]) and used in the proof of Thm. 5.3, the soundness of d-separation for a 3-place relation on subsets of nodes can be established by showing that the relation satisfies the *local Markov condition* and the *semi-graphoid axioms*.

In order to see that the local Markov condition holds, let $X \in V$ and define $P := Pa(X)$ and $N := Nd(X) \setminus Pa(X)$. The nodes in $D = V \backslash (\{X\} \cup P \cup N)$ are the descendants of X. Without any further partitioning of sets, Fig. A.3 is already of the required form, hence $SR(\{X\}, N; P)$.

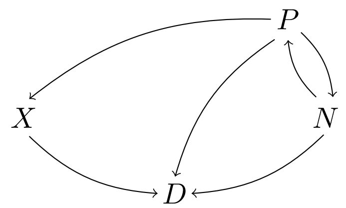


Figure A.3: $SR(\{X\}, N; P)$.

Now consider the semi-graphoid axioms. The symmetry axiom $SR(Y, Z; W) \Leftrightarrow SR(Z, Y; W)$ is immediate. Concerning the decomposition axiom, $SR(Y, XZ; W) \Rightarrow SR(Y, Z; W)$, suppose that $SR(Y, XZ; W)$ holds, with corresponding decompositions $W = W_Y \cup W_{XZ}$ and $R = R_Y \cup R_{XZ} \cup R^c$. Defining $R_Z := R_{XZ} \cup X$ and $W_Z := W_{XZ}$, it follows immediately that $SR(Y, Z; W)$ holds, with corresponding decompositions $W = W_Y \cup W_Z$ and $R = R_Y \cup R_Z \cup R^c$. Concerning the weak union axiom, $SR(Y, XZ; W) \Rightarrow SR(Y, Z; XW)$, suppose that $SR(Y, XZ; W)$ holds, with corresponding decompositions $W = W_Y \cup W_{XZ}$ and $R = R_Y \cup R_{XZ} \cup R^c$. Defining $W_Z := W_{XZ} \cup X$ and $R_Z := R_{XZ}$, it is immediate that $SR(Y, Z; XW)$ holds with corresponding decompositions $X \cup W = W_Y \cup W_Z$ and $R = R_Y \cup R_Z \cup R^c$. Finally, concerning the contraction axiom, suppose that $SR(Y, Z; W) \wedge SR(Y, X; ZW)$.

Let the subsets implied by these two relations be labelled as in Figs. A.4 and A.5.

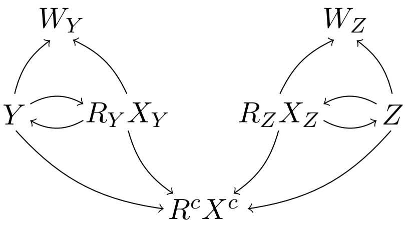


Figure A.4: $SR(Y, Z; W)$.

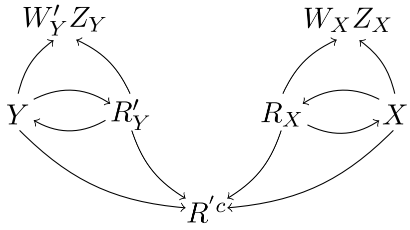


Figure A.5: $SR(Y, X; ZW)$.

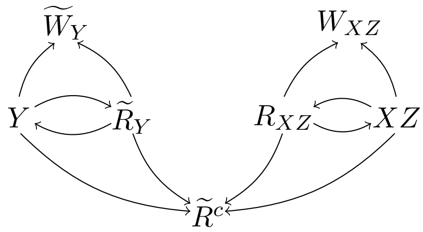


Figure A.6: $SR(Y, ZX; W)$.

Defining new sets as follows,

$$\begin{aligned} W_{XZ} &:= W_X \cup W_Z \\ \widetilde{W}_Y &:= W \setminus W_{XZ} \end{aligned} \qquad \begin{aligned} R_{XZ} &:= R_X \cup R_Z \\ \widetilde{R}^c &:= (R^c \cup R'^c) \setminus R_{XZ} \\ \widetilde{R}_Y &:= R \setminus (R_{XZ} \cup \widetilde{R}^c) \ , \end{aligned}$$

the diagram in Fig. A.6 correctly expresses which parent-child relations between those subsets are forbidden, i.e. there must not be any arrows from R_{XZ}, X or Z to the sets on the left and no arrows from $\widetilde{R}_Y$ or Y to any sets on the right. This establishes $SR(Y, ZX; W)$. □

A.5 Proof of Proposition 5.2

The only if direction is immediate.

For the if direction, consider an informationally complete intervention at each node $A \in Y$: that is, an intervention corresponding to a quantum instrument $\{\tau_A^{k_A}\}$ such that, varying over k_A, the operators $\tau_A^{k_A}$ span the real vector space of Hermitian operators on $\mathcal{H}_{A^{\text{in}}} \otimes \mathcal{H}^*_{A^{\text{out}}}$. Let k_Y denote the joint outcome, and for each k_Y, let $\tau_Y^{k_Y}$ denote the corresponding tensor product of local operators. Varying over k_Y, the operators $\tau_Y^{k_Y}$ span the real vector space of Hermitian operators on $\mathcal{H}_{Y^{\text{in}}} \otimes \mathcal{H}^*_{Y^{\text{out}}}$, i.e., the local intervention at Y, consisting of a product of informationally complete interventions, is also informationally complete. Similarly, consider an informationally complete local intervention at Z, with joint outcome k_Z, and corresponding product operators $\tau_Z^{k_Z}$.

Given σ_{YZ}, suppose that $P(k_Y, k_Z) = \mathrm{Tr}_{YZ}[\sigma_{YZ}(\tau_Y^{k_Y} \otimes \tau_Z^{k_Z})] = P(k_Y)P(k_Z)$. Let α_Y be the operator such that $P(k_Y) = \mathrm{Tr}_Y(\alpha_Y \tau_Y^{k_Y})$ and β_Z be the operator such that $P(k_Z) = \mathrm{Tr}_Z(\beta_Z \tau_Z^{k_Z})$. Since $\{\tau_Y^{k_Y} \otimes \tau_Z^{k_Z}\}_{k_Y,k_Z}$ spans the tensor product space of operators, σ_{YZ} and $\alpha_Y \otimes \beta_Z$ agree on a basis, hence $\sigma_{YZ} = \alpha_Y \otimes \beta_Z = \sigma_Y \otimes \sigma_Z$. □

A.6 Proof of Proposition 5.5

For the only if direction, assume that $(Y \perp\!\!\!\perp Z|W)_\kappa$ holds, hence κ_{YZW} can be written in the form $\kappa_{YZW} = \alpha_{YW}\beta_{ZW}$. Consider arbitrary interventions at Y and Z, and a maximally informative intervention at W. Then by Def. 5.13, functions g^{in} and g^{out} exist such that

$$\begin{aligned} P(k_Y, k_Z, k_W) &= \sum_Y \sum_Z \sum_W \kappa_{YZW}\ P(k_Y, Y^{\text{out}}|Y^{\text{in}})\ P(k_Z, Z^{\text{out}}|Z^{\text{in}}) \\ &\qquad \delta(g^{\text{in}}(k_W), W^{\text{in}})\ \delta(g^{\text{out}}(k_W), W^{\text{out}})\ P(k_W, W^{\text{out}}|W^{\text{in}}) \\ &= \sum_Y \alpha_{YW}(Y^{\text{in}}, Y^{\text{out}}, g^{\text{in}}(k_W), g^{\text{out}}(k_W))\ P(k_Y, Y^{\text{out}}|Y^{\text{in}}) \\ &\quad \sum_Z \beta_{ZW}(Z^{\text{in}}, Z^{\text{out}}, g^{\text{in}}(k_W), g^{\text{out}}(k_W))\ P(k_Z, Z^{\text{out}}|Z^{\text{in}}) \\ &\qquad P(k_W, g^{\text{out}}(k_W)|g^{\text{in}}(k_W))\ . \end{aligned}$$

Setting

$$\alpha'(k_Y, k_W) = \sum_Y \alpha_{YW}(Y^{\text{in}}, Y^{\text{out}}, g^{\text{in}}(k_W), g^{\text{out}}(k_W))\ P(k_Y, Y^{\text{out}}|Y^{\text{in}}),$$

and

$$\begin{aligned} \beta'(k_Z, k_W) &= \sum_Z \beta_{ZW}(Z^{\text{in}}, Z^{\text{out}}, g^{\text{in}}(k_W), g^{\text{out}}(k_W))\ P(k_Z, Z^{\text{out}}|Z^{\text{in}}) \\ &\qquad P(k_W, g^{\text{out}}(k_W)|g^{\text{in}}(k_W)) \end{aligned}$$

yields $P(k_Y, k_Z, k_W) = \alpha'(k_Y, k_W)\beta'(k_Z, k_W)$, hence $(k_Y \perp\!\!\!\perp k_Z|k_W)_P$, by Prop. 5.3.

For the if direction, assume that for any local interventions at Y and Z, and any maximally informative local intervention at W, the joint outcome probabilities $P(k_Y, k_Z, k_W)$ satisfy $(k_Y \perp\!\!\!\perp k_Z|k_W)_P$. Consider, in particular, an intervention at each node X (where $X \in Y$, $X \in Z$, or $X \in W$), such that the outcome k_X is a pair $k_X = (k_X^I, k_X^O)$, and

$$P(k_X, X^{\text{out}}|X^{\text{in}}) = \frac{1}{d_X}\delta(k_X^I, X^{\text{in}})\delta(k_X^O, X^{\text{out}}),$$

where d_X is the cardinality of the set on which X^{in} takes values. This corresponds to measuring the input variable, recording the value as k_X^I, choosing a value k_X^O at random, and setting $X^{\text{out}} = k_X^O$. Assume that the local intervention at Y is a product of interventions of this form, with joint outcome $k_Y = (k_Y^I, k_Y^O)$, where k_Y^I is the tuple consisting of a value of k_X^I, for each $X \in Y$, and k_Y^O is the tuple consisting of a value of k_X^O, for each $X \in Y$. Similarly Z and $k_Z = (k_Z^I, k_Z^O)$, and W and $k_W = (k_W^I, k_W^O)$. Observe that these interventions are maximally informative, in keeping with the assumption of a maximally informative intervention at W.

Given $(k_Y \perp\!\!\!\perp k_Z|k_W)_P$, it follows from Prop. 5.3 that there exist $\alpha(k_Y, k_W)$ and $\beta(k_Z, k_W)$ such that $P(k_Y, k_Z, k_W) = \alpha(k_Y, k_W)\beta(k_Z, k_W)$. Define $\alpha'_{YW} : Y^{\text{in}} \times Y^{\text{out}} \times W^{\text{in}} \times W^{\text{out}} \to \mathbb{R}$ and $\beta'_{ZW} : Z^{\text{in}} \times Z^{\text{out}} \times W^{\text{in}} \times W^{\text{out}} \to \mathbb{R}$ such that

$$\begin{aligned}
\alpha'_{YW}(Y^{\text{in}}, Y^{\text{out}}, W^{\text{in}}, W^{\text{out}}) &= d_Y d_W\ \alpha(k_Y, k_W)\big|_{k_Y=(Y^{\text{in}},Y^{\text{out}}),k_W=(W^{\text{in}},W^{\text{out}})}\ , \\
\beta'_{ZW}(Z^{\text{in}}, Z^{\text{out}}, W^{\text{in}}, W^{\text{out}}) &= d_Z\ \beta(k_Z, k_W)\big|_{k_Z=(Z^{\text{in}},Z^{\text{out}}),k_W=(W^{\text{in}},W^{\text{out}})}\ .
\end{aligned}$$

Observe that

$$\begin{aligned}
\alpha(k_Y, k_W) &= \sum_{YW} \alpha'_{YW} P(k_Y, Y^{\text{out}}|Y^{\text{in}}) P(k_W, W^{\text{out}}|W^{\text{in}})\ , \\
\beta(k_Z, k_W) &= d_W \sum_{ZW} \beta'_{ZW} P(k_Z, Z^{\text{out}}|Z^{\text{in}}) P(k_W, W^{\text{out}}|W^{\text{in}})\ .
\end{aligned}$$

Now,

$$\begin{aligned}
P(k_Y, k_Z, k_W) &= \alpha(k_Y, k_W)\ \beta(k_Z, k_W) \\
&= d_W \Big(\sum_{YW} \alpha'_{YW}\ P(k_Y, Y^{\text{out}}|Y^{\text{in}})\ P(k_W, W^{\text{out}}|W^{\text{in}})\Big) \\
&\qquad \Big(\sum_{ZW} \beta'_{ZW}\ P(k_Z, Z^{\text{out}}|Z^{\text{in}})\ P(k_W, W^{\text{out}}|W^{\text{in}})\Big) \\
&= \sum_{YZW} \alpha'_{YW}\ \beta'_{ZW}\ P(k_Y, Y^{\text{out}}|Y^{\text{in}})\ P(k_Z, Z^{\text{out}}|Z^{\text{in}}) \\
&\qquad P(k_W, W^{\text{out}}|W^{\text{in}})\ ,
\end{aligned} \tag{A.23}$$

where the third equality follows from the form of the W intervention (in particular, the fact that the W intervention is maximally informative). From the definition of the classical process map,

$$P(k_Y, k_Z, k_W) = \sum_{YZW} \kappa_{YZW} \; P(k_Y, Y^{\text{out}}|Y^{\text{in}}) \; P(k_Z, Z^{\text{out}}|Y^{\text{in}}) \; P(k_W, W^{\text{out}}|W^{\text{in}}) \; . \tag{A.24}$$

The measurements considered are informationally complete: that is, if for fixed k_Y, k_Z, k_W, the term $P(k_Y, Y^{\text{out}}|Y^{\text{in}})P(k_Z, Z^{\text{out}}|Z^{\text{in}})P(k_W, W^{\text{out}}|W^{\text{in}})$ is viewed as a real-valued function of Y^{in}, Y^{out}, Z^{in}, Z^{out}, W^{in}, W^{out}, then, varying over k_Y, k_Z, k_W, these functions span the vector space of all real-valued functions of Y^{in}, Y^{out}, Z^{in}, Z^{out}, W^{in}, W^{out}. Comparing Eqs. (A.23) and (A.24) then gives $\kappa_{YZW} = \alpha'_{YW}\beta'_{ZW}$, that is $(Y \perp\!\!\!\perp Z|W)_{\kappa_{YZW}}$. □

A.7 Proof of Lemmas 5.2 and 5.3

Proof of Lemma 5.2. Let σ_V be a process operator, and consider the relation T of Eq. (5.27), defined over triples of disjoint subsets of V. The symmetry axiom from Eq. (5.21) is immediate. For the decomposition axiom from Eq. (5.22), suppose that $T(Y, XZ; W)$ holds, i.e., for all local interventions τ^R, there exist α_{YW} and β_{XZW} such that $\sigma^{\tau_R}_{YXZW} = \alpha_{YW} \; \beta_{XZW}$. Then for any choice of local intervention τ_X at X, $\sigma^{\tau_R\tau_X}_{YZW} = \alpha_{YW} \; \text{Tr}_X\left[\tau_X \beta_{XZW}\right]$, hence $(Y \perp\!\!\!\perp Z|W)_{\sigma^{\tau_R\tau_X}_{YZW}}$, hence $T(Y, Z; W)$ holds. The weak union axiom from Eq. (5.23) is immediate. Finally, for the contraction axiom from Eq. (5.24), suppose that for all local interventions τ_R and τ_X, $(Y \perp\!\!\!\perp Z|W)_{\sigma^{\tau_R\tau_X}_{YZW}}$, and that for all local interventions τ_R, $(Y \perp\!\!\!\perp X|ZW)_{\sigma^{\tau_R}_{YXZW}}$. The first condition, along with Part (3) of Prop. 5.7, implies that for all local interventions τ_R and τ_X, the quantum conditional mutual information $I(Y : Z|W) = 0$ when evaluated on $\hat{\sigma}^{\tau_R\tau_X}_{YZW}$. Similarly, the second condition implies that for all local interventions τ_R, $I(Y : X|ZW) = 0$ when evaluated on $\hat{\sigma}^{\tau_R}_{YZWX}$.[1] Let τ_X be the intervention that, at each node in X, ignores the input and prepares a maximally mixed state on the output. This yields

$$\begin{aligned} H(\text{Tr}_{ZX}[\hat{\sigma}^{\tau_R}_{YZWX}]) + H(\text{Tr}_{YX}[\hat{\sigma}^{\tau_R}_{YZWX}]) \qquad & \\ -H(\text{Tr}_{YZX}[\hat{\sigma}^{\tau_R}_{YZWX}]) - H(\text{Tr}_{X}[\hat{\sigma}^{\tau_R}_{YZWX}]) &= 0 \\ H(\text{Tr}_{X}[\hat{\sigma}^{\tau_R}_{YZWX}]) + H(\text{Tr}_{Y}[\hat{\sigma}^{\tau_R}_{YZWX}]) - H(\text{Tr}_{YX}[\hat{\sigma}^{\tau_R}_{YZWX}]) - H(\hat{\sigma}^{\tau_R}_{YZWX}) &= 0 \end{aligned}$$

where $H(...)$ denotes the von Neumann entropy. Adding the two equations gives

[1]The following steps are essentially the same as those used in Ref. [76] to show that the condition $I(A : B|C) = 0$ on ordinary quantum states satisfies the semi-graphoid axioms.

$I(Y : XZ|W) = 0$, when evaluated on $\hat{\sigma}^{\tau_R}_{YZWX}$. Seeing as this holds for any local intervention τ_R, Prop. 5.7 gives $T(Y, XZ; W)$. □

Proof of Lemma 5.3. Consider a DAG G, with nodes V, and a process operator σ_V, such that σ_V is Markov for G. Let $X \in V$ and set $P := Pa(X)$, $N := Nd(X) \setminus Pa(X)$ and $D := V \setminus (X \cup P \cup N)$. The sets $\{X\}$, P, N and D constitute a partition of V, hence $\sigma_V = \rho_{X|Pa(X)}\ \rho_{P|Pa(P)}\ \rho_{N|Pa(N)}\ \rho_{D|Pa(D)}$. The set D only contains descendants of X, hence D cannot have children in any of the other sets. Given an arbitrary local intervention τ_D, the marginal process operator over XPN is therefore of the form $\sigma^{\tau_D}_{XPN} = \mathrm{Tr}_D[\sigma_{XPND}\ \tau_D] = \rho_{X|Pa(X)}\ \rho_{P|Pa(P)}\ \rho_{N|Pa(N)}$. By definition, $X \notin P$ and $N \cap P = \emptyset$, hence $\sigma^{\tau_D}_{XPN}$ is of the form $\alpha_{XP}\ \beta_{NP}$, with $\alpha_{XP} = \rho_{X|Pa(X)}$ and $\beta_{NP} = \rho_{P|Pa(P)}\ \rho_{N|Pa(N)}$. Therefore $T(X, N; P)$ holds. □

A.8 Proof of Proposition 5.9

This is essentially the same as the proof of Prop. 5.6, except that with $\sigma_{YZWdo(X)} = \alpha_{YWX^{\mathrm{out}}}\ \beta_{ZWX^{\mathrm{out}}}$, the two factors have non-trivial action on the three Hilbert spaces $\mathcal{H}_{W^{\mathrm{in}}}$, $\mathcal{H}^*_{W^{\mathrm{out}}}$ and $\mathcal{H}^*_{X^{\mathrm{out}}}$. The relevant decomposition into orthogonal subspaces that follows from Lem. 4.1, is therefore a decomposition of $\mathcal{H}_{W^{\mathrm{in}}} \otimes \mathcal{H}^*_{W^{\mathrm{out}}} \otimes \mathcal{H}^*_{X^{\mathrm{out}}}$. The proof proceeds with 'WX^{out}' replacing W. □

A.9 Proof of Proposition 5.10

(1) → (2)

Suppose that $\sigma_{YZWdo(X)} = \alpha_{YWX^{\mathrm{out}}}\beta_{ZWX^{\mathrm{out}}}$ for a pair of Hermitian operators $\alpha_{YWX^{\mathrm{out}}}$ and $\beta_{ZWX^{\mathrm{out}}}$. Taking the Hermitian conjugate of both sides of this equation establishes that $[\alpha_{YWX^{\mathrm{out}}}, \beta_{ZWX^{\mathrm{out}}}] = 0$. For arbitrary local interventions τ_Y at Y and τ_Z at Z, let $\alpha^{\tau_Y}_{WX^{\mathrm{out}}} = \mathrm{Tr}_Y\left[\alpha_{YWX^{\mathrm{out}}}\ \tau_Y\right]$ and $\beta^{\tau_Z}_{WX^{\mathrm{out}}} = \mathrm{Tr}_Z\left[\beta_{ZWX^{\mathrm{out}}}\ \tau_Z\right]$. Observe that $[\alpha^{\tau_Y}_{WX^{\mathrm{out}}}, \beta_{ZWX^{\mathrm{out}}}] = 0$ and $[\alpha_{YWX^{\mathrm{out}}}\ ,\ \beta^{\tau_Z}_{WX^{\mathrm{out}}}] = 0$

Using the commutativity and associativity of the '$\star$'-product, along with the fact that for arbitrary Hermitian operators M and N, if $[M, N] = 0$ then $M \star N = MN$,

$$\begin{aligned}
\sigma_{YZWdo(X)} \star \sigma^{\tau_Y,\tau_Z}_{Wdo(X)} &= \left(\alpha_{YWX^{\mathrm{out}}}\ \beta_{ZWX^{\mathrm{out}}}\right) \star \left(\alpha^{\tau_Y}_{WX^{\mathrm{out}}}\ \beta^{\tau_Z}_{WX^{\mathrm{out}}}\right) \\
&= \alpha_{YWX^{\mathrm{out}}} \star \beta_{ZWX^{\mathrm{out}}} \star \alpha^{\tau_Y}_{WX^{\mathrm{out}}} \star \beta^{\tau_Z}_{WX^{\mathrm{out}}} \\
&= \left(\alpha_{YWX^{\mathrm{out}}}\ \beta^{\tau_Z}_{WX^{\mathrm{out}}}\right) \star \left(\alpha^{\tau_Y}_{WX^{\mathrm{out}}}\ \beta_{ZWX^{\mathrm{out}}}\right) \\
&= \sigma^{\tau_Z}_{YWdo(X)} \star \sigma^{\tau_Y}_{ZWdo(X)}\ .
\end{aligned}$$

(2) → (3)

Assume (2), and consider local interventions τ_Y and τ_Z that consist of discarding the input, and preparing a maximally mixed state on the output, for each node in the corresponding set. Dividing each side of (2) by $d_Y d_Z (d_W d_X)^2$, and taking logarithms, gives

$$\log\Big(\hat{\sigma}_{YZWdo(X)}\Big) \ + \ \log\Big(\mathrm{Tr}_{YZ}(\hat{\sigma}_{YZWdo(X)})\Big) \\ = \ \log\Big(\mathrm{Tr}_Z(\hat{\sigma}_{YZWdo(X)})\Big) \ + \ \log\Big(\mathrm{Tr}_Y(\hat{\sigma}_{YZWdo(X)})\Big),$$

where the logarithms are restricted to the support of the respective operators. This implies (3).

(3) → (1)

Assume (3). By Theorem 6 of Ref. [122], there is a decomposition of the form $\mathcal{H}_{W^{\mathrm{in}}} \otimes \mathcal{H}^*_{W^{\mathrm{out}}} \otimes \mathcal{H}^*_{X^{\mathrm{out}}} = \bigoplus_i \mathcal{H}_{(WX^{\mathrm{out}})^L_i} \otimes \mathcal{H}_{(WX^{\mathrm{out}})^R_i}$, and a probability distribution $\{p_i\}$ such that $\hat{\sigma}_{YZWdo(X)} = \sum_i p_i \ \hat{\sigma}_{Y(WX^{\mathrm{out}})^L_i} \otimes \hat{\sigma}_{Z(WX^{\mathrm{out}})^R_i}$ for positive trace-1 operators $\hat{\sigma}_{Y(WX^{\mathrm{out}})^L_i}$ and $\hat{\sigma}_{Z(WX^{\mathrm{out}})^R_i}$. Define Hermitian operators

$$\alpha_{YWX^{\mathrm{out}}} \ := \ d_Y d_Z d_W d_X \sum_i p_i \ \hat{\sigma}_{Y(WX^{\mathrm{out}})^L_i} \otimes \mathbb{1}_{Z(WX^{\mathrm{out}})^R_i} \ , \tag{A.25}$$

$$\beta_{ZWX^{\mathrm{out}}} \ := \ \sum_i \mathbb{1}_{Y(WX^{\mathrm{out}})^L_i} \otimes \hat{\sigma}_{Z(WX^{\mathrm{out}})^R_i} \ . \tag{A.26}$$

Since the distinct subspaces are orthogonal, $\sigma_{YZWdo(X)} = \alpha_{YWX^{\mathrm{out}}}\beta_{ZWX^{\mathrm{out}}}$, which establishes the claim. □

A.10 Proof of Theorem 5.5

Let σ_{YZWXR} be a process operator that is Markov for G, hence $\sigma_{YZWRdo(X)} = \rho_{Y|Pa(Y)} \ \rho_{Z|Pa(Z)} \ \rho_{W|Pa(W)} \ \rho_{R|Pa(R)}$, where all operators commute and may act non-trivially on $\mathcal{H}^*_{X^{\mathrm{out}}}$. Suppose that $(Y \perp\!\!\!\perp Z|WX)_{G_{\overline{X}}}$. Recalling Def. A.1, Lem. A.2 implies that $SR(Y,Z;WX)$ holds in $G_{\overline{X}}$. Therefore there exist partitions $R = R_Y \cup R_Z \cup R^c$ and $W \cup X = W_Y \cup X_Y \cup W_Z \cup X_Z$, with

$$\rho_{W|Pa(W)} = \rho_{W_Y|Pa(W_Y)} \ \rho_{W_Z|Pa(W_Z)}$$

and

$$\rho_{R|Pa(R)} = \rho_{R_Y|Pa(R_Y)} \ \rho_{R_Z|Pa(R_Z)} \ \rho_{R^c|Pa(R^c)}$$

such that each of the operators $\rho_{Y|Pa(Y)}$, $\rho_{W_Y|Pa(W_Y)}$, $\rho_{R_Y|Pa(R_Y)}$ acts trivially on the input and (the duals of the) output spaces of the nodes in $Z \cup R_Z \cup R^c$, and each of the operators $\rho_{Z|Pa(Z)}$, $\rho_{W_Z|Pa(W_Z)}$, $\rho_{R_Z|Pa(R_Z)}$ acts trivially on the input and (the duals of the) output spaces of the nodes in $Y \cup R_Y \cup R^c$. With $\tau_R = \tau_{R_Y} \otimes \tau_{R_Z} \otimes \tau_{R^c}$ an arbitrary local intervention at R, the term $\mathrm{Tr}_{R^c}[\rho_{R^c|Pa(R^c)}\ \tau_{R^c}] = \mathbb{1}$ (identity on the duals of the output spaces of $Pa(R^c) \setminus R^c$) , and it follows that

$$\sigma^{\tau_R}_{YZWdo(X)} = \mathrm{Tr}_R \left[\ \tau_R\ \sigma_{YZWRdo(X)}\ \right] = \mathrm{Tr}_{R_Y} \left[\ \tau_{R_Y}\ \rho_{Y|Pa(Y)}\ \rho_{W_Y|Pa(W_Y)}\ \rho_{R_Y|Pa(R_Y)}\right] \mathrm{Tr}_{R_Z} \left[\ \tau_{R_Z}\ \rho_{Z|Pa(Z)}\ \rho_{W_Z|Pa(W_Z)}\ \rho_{R_Z|Pa(R_Z)}\ \right].$$

Setting

$$\alpha_{YWX^{\mathrm{out}}} = \mathrm{Tr}_{R_Y} \left[\ \tau_{R_Y}\ \rho_{Y|Pa(Y)}\ \rho_{W_Y|Pa(W_Y)}\ \rho_{R_Y|Pa(R_Y)}\right]$$

and

$$\beta_{ZWX^{\mathrm{out}}} = \mathrm{Tr}_{R_Z} \left[\ \tau_{R_Z}\ \rho_{Z|Pa(Z)}\ \rho_{W_Z|Pa(W_Z)}\ \rho_{R_Z|Pa(R_Z)}\ \right]$$

concludes the proof. □

A.11 Proof of Proposition 5.11

$(Y \perp\!\!\!\perp Z^{\mathrm{in}}|W do(X) Z^{\mathrm{out}})_{\kappa_{YZWX}} \Rightarrow$ (COS2):

Let κ_{YZWX} represent a classical process map, and suppose that $\kappa_{YZWdo(X)} = \alpha_{YWX^{\mathrm{out}}Z^{\mathrm{out}}}\ \beta_{ZWX^{\mathrm{out}}}$, for suitable functions $\alpha_{YWX^{\mathrm{out}}Z^{\mathrm{out}}}$ and $\beta_{ZWX^{\mathrm{out}}}$. Then, for an arbitrary local intervention at Y, a breaking local intervention at Z that fixes $Z^{\mathrm{out}} = z$, a maximally informative local intervention at W, and a do-intervention that fixes $X^{\mathrm{out}} = x$,

$$\begin{aligned} P(k_Y, k_Z, k_W) &= \sum_{Y,Z,W} \sum_{X^{\mathrm{out}}} \Big[\ \kappa_{YZWdo(X)}\ P(k_Y, Y^{\mathrm{out}}|Y^{\mathrm{in}}) \\ &\qquad \delta(X^{\mathrm{out}}, x)\ \delta(Z^{\mathrm{out}}, z)\ P(k_Z|Z^{\mathrm{in}}) \\ &\qquad \delta\Big(g^{\mathrm{in}}(k_W), W^{\mathrm{in}}\Big)\ \delta\Big(g^{\mathrm{out}}(k_W), W^{\mathrm{out}}\Big)\ P(k_W, W^{\mathrm{out}}|W^{\mathrm{in}})\ \Big] \\ &= \Big(\sum_Y\ P(k_Y, Y^{\mathrm{out}}|Y^{\mathrm{in}})\, \alpha_{YWX^{\mathrm{out}}Z^{\mathrm{out}}}\left(Y^{\mathrm{in}}, Y^{\mathrm{out}}, g^I(k_W), g^O(k_W), x, z\right)\Big) \\ &\quad \Big(\sum_{Z^{\mathrm{in}}} P(k_Z|Z^{\mathrm{in}}) P(k_W, g^{\mathrm{out}}(k_W)|g^{\mathrm{in}}(k_W))\, \beta_{ZWX^{\mathrm{out}}}\left(Z^{\mathrm{in}}, z, g^I(k_W), g^O(k_W), x\right)\Big). \end{aligned}$$

Setting

$$\alpha'(k_Y, k_W) = \sum_Y\ P(k_Y, Y^{\mathrm{out}}|Y^{\mathrm{in}})\, \alpha_{YWX^{\mathrm{out}}Z^{\mathrm{out}}}\left(Y^{\mathrm{in}}, Y^{\mathrm{out}}, g^I(k_W), g^O(k_W), x, z\right),$$

and

$$\beta'(k_Z, k_W) = \sum_{Z^{\text{in}}} P(k_Z|Z^{\text{in}})\ P(k_W, g^{\text{out}}(k_W)|g^{\text{in}}(k_W)) \\ \beta_{ZWX^{\text{out}}}\left(Z^{\text{in}}, z, g^I(k_W), g^O(k_W), x\right),$$

yields $P(k_Y, k_Z, k_W) = \alpha'(k_Y, k_W)\beta'(k_Z, k_W)$, hence $(k_Y \perp\!\!\!\perp k_Z|k_W)_P$, by Prop. 5.3.

(COS2) $\Rightarrow (Y \perp\!\!\!\perp Z^{\text{in}}|W do(X) Z^{\text{out}})_{\kappa_{YZWX}}$:

The converse direction proceeds by a similar argument to that of the proof of Prop. 5.5. Consider an intervention at each node N (where $N \in Y$ or $N \in W$), such that the outcome k_N is a pair $k_N = (k_N^I, k_N^O)$, and

$$P(k_N, N^{\text{out}}|N^{\text{in}}) = \frac{1}{d_N}\delta(k_N^I, N^{\text{in}})\delta(k_N^O, N^{\text{out}}),$$

where d_N is the cardinality of the set on which N^{out} takes values. Assume that the local intervention at Y is a product of interventions of this form, with joint outcome $k_Y = (k_Y^I, k_Y^O)$, where k_Y^I is the tuple consisting of a value of k_N^I, for each $N \in Y$, and k_Y^O is the tuple consisting of a value of k_N^O, for each $N \in Y$. Similarly W and $k_W = (k_W^I, k_W^O)$. Consider a breaking local intervention at Z that fixes $Z^{\text{out}} = z$, and returns $k_Z = Z^{\text{in}}$. Consider a do-intervention at X that fixes $X^{\text{out}} = x$.

For each choice of (x, z), let $P_{xz}(k_Y, k_Z, k_W)$ be the joint distribution over outcomes, and assume that the condition $(k_Y \perp\!\!\!\perp k_Z|k_W)_{P_{xz}}$ holds. It follows from Prop. 5.3 that there exist $\alpha_{xz}(k_Y, k_W)$ and $\beta_{xz}(k_Z, k_W)$ such that $P_{xz}(k_Y, k_Z, k_W) = \alpha_{xz}(k_Y, k_W)\beta_{xz}(k_Z, k_W)$. Define $\alpha'_{YWX^{\text{out}}Z^{\text{out}}} : Y^{\text{in}} \times Y^{\text{out}} \times W^{\text{in}} \times W^{\text{out}} \times X^{\text{out}} \times Z^{\text{out}} \to \mathbb{R}$ and $\beta'_{ZWX^{\text{out}}} : Z^{\text{in}} \times Z^{\text{out}} \times W^{\text{in}} \times W^{\text{out}} \times X^{\text{out}} \to \mathbb{R}$ such that for each x, z,

$$\alpha'_{YWX^{\text{out}}Z^{\text{out}}}(Y^{\text{in}}, Y^{\text{out}}, W^{\text{in}}, W^{\text{out}}, x, z) = d_Y d_W\ \alpha_{xz}(k_Y, k_W)\big|_{k_Y=(Y^{\text{in}},Y^{\text{out}}),k_W=(W^{\text{in}},W^{\text{out}})},$$
$$\beta'_{ZWX^{\text{out}}}(Z^{\text{in}}, z, W^{\text{in}}, W^{\text{out}}, x) = \beta_{xz}(k_Z, k_W)\big|_{k_Z=Z^{\text{in}},k_W=(W^{\text{in}},W^{\text{out}})}.$$

Observe that

$$\alpha_{xz}(k_Y, k_W) = \sum_{YW} \alpha'_{YWX^{\text{out}}Z^{\text{out}}}(Y^{\text{in}}, Y^{\text{out}}, W^{\text{in}}, W^{\text{out}}, x, z) \\ P(k_Y, Y^{\text{out}}|Y^{\text{in}})\ P(k_W, W^{\text{out}}|W^{\text{in}}),$$
$$\beta_{xz}(k_Z, k_W) = d_W \sum_{Z^{\text{in}}W} \beta'_{ZWX^{\text{out}}}(Z^{\text{in}}, z, W^{\text{in}}, W^{\text{out}}, x)\ P(k_Z|Z^{\text{in}})\ P(k_W, W^{\text{out}}|W^{\text{in}}).$$

Now,

$$
\begin{aligned}
P_{xz}(k_Y, k_Z, k_W) &= \alpha_{xz}(k_Y, k_W)\beta_{xz}(k_Z, k_W) \\
&= d_W\Big(\sum_{YW} \alpha'_{YWX^{\text{out}}Z^{\text{out}}}(Y^{\text{in}}, Y^{\text{out}}, W^{\text{in}}, W^{\text{out}}, x, z) \\
&\qquad\qquad P(k_Y, Y^{\text{out}}|Y^{\text{in}})P(k_W, W^{\text{out}}|W^{\text{in}})\Big) \\
&\quad \Big(\sum_{Z^{\text{in}}W} \beta'_{ZWX^{\text{out}}}(Z^{\text{in}}, z, W^{\text{in}}, W^{\text{out}}, x)P(k_Z|Z^{\text{in}})P(k_W, W^{\text{out}}|W^{\text{in}})\Big) \\
&= \sum_{YZ^{\text{in}}W} P(k_Y, Y^{\text{out}}|Y^{\text{in}})\ P(k_Z|Z^{\text{in}})\ P(k_W, W^{\text{out}}|W^{\text{in}}) \\
&\qquad\qquad (\alpha'_{YWX^{\text{out}}Z^{\text{out}}}\ \beta'_{ZWX^{\text{out}}})\big|_{X^{\text{out}}=x, Z^{\text{out}}=z} \\
&= \sum_{YZW} P(k_Y, Y^{\text{out}}|Y^{\text{in}})\ P(k_Z, Z^{\text{out}}|Z^{\text{in}})P(k_W, W^{\text{out}}|W^{\text{in}}) \\
&\qquad\qquad (\alpha'_{YWX^{\text{out}}Z^{\text{out}}}\ \beta'_{ZWX^{\text{out}}})\big|_{X^{\text{out}}=x},
\end{aligned} \tag{A.27}
$$

where the third equality follows from the form of the W intervention (in particular, the fact that the W intervention is maximally informative), and where

$$P(k_Z, Z^{\text{out}}|Z^{\text{in}}) = P(k_Z|Z^{\text{in}})\delta(Z^{\text{out}}, z).$$

From the definition of the do-conditional process map,

$$
\begin{aligned}
P_{xz}(k_Y, k_Z, k_W) &= \sum_{YZW} P(k_Y, Y^{\text{out}}|Y^{\text{in}})\ P(k_Z, Z^{\text{out}}|Z^{\text{in}})\ P(k_W, W^{\text{out}}|W^{\text{in}}) \\
&\qquad\qquad \big(\kappa_{YZWdo(X)}\big)\big|_{X^{\text{out}}=x}.
\end{aligned} \tag{A.28}
$$

The measurements considered are informationally complete: that is, if for fixed z, k_Y, k_Z, k_W, the term $P(k_Y, Y^{\text{out}}|Y^{\text{in}})P(k_Z, Z^{\text{out}}|Z^{\text{in}})P(k_W, W^{\text{out}}|W^{\text{in}})$ is viewed as a real-valued function of Y^{in}, Y^{out}, Z^{in}, Z^{out}, W^{in}, W^{out}, then, varying over z, k_Y, k_Z, k_W, these functions span the vector space of all real-valued functions of Y^{in}, Y^{out}, Z^{in}, Z^{out}, W^{in}, W^{out}. Comparing Eqs. (A.27) and (A.28) yields $\kappa_{YZWdo(X)} = \alpha'_{YWX^{\text{out}}}\beta'_{ZWX^{\text{out}}}$, that is $(Y \perp\!\!\!\perp Z^{\text{in}}|Wdo(X)Z^{\text{out}})_{\kappa_{YZWX}}$. □

A.12 Proof of Proposition 5.12

The proof is similar to that of Prop. 5.6 (and Prop. 5.9).

Assume $(Y \perp\!\!\!\perp Z^{\text{in}}|Wdo(X)Z^{\text{out}})_{\sigma_{YZWX}}$, hence there exist Hermitian operators $\alpha_{YWX^{\text{out}}Z^{\text{out}}}$ and $\beta_{ZWX^{\text{out}}}$ such that $\sigma_{YZWdo(X)} = \alpha_{YWX^{\text{out}}Z^{\text{out}}}\ \beta_{ZWX^{\text{out}}}$. Lem. 4.1 implies that there is a decomposition $\mathcal{H}_{W^{\text{in}}}\otimes\mathcal{H}^*_{W^{\text{out}}}\otimes\mathcal{H}^*_{X^{\text{out}}}\otimes\mathcal{H}^*_{Z^{\text{out}}} = \bigoplus_i \mathcal{H}_{F_i^L}\otimes\mathcal{H}_{F_i^R}$ such that $\sigma_{YZWdo(X)} = \sum_i \alpha_{YF_i^L}\otimes\beta_{Z^{\text{in}}F_i^R}$, with $\alpha_{YF_i^L}$ and $\beta_{Z^{\text{in}}F_i^R}$ positive for all i. Let

$\{|i, f_i^L\rangle\, |i, f_i^R\rangle\}_{f_i^L, f_i^R}$ be a product orthonormal basis of the ith subspace $\mathcal{H}_{F_i^L} \otimes \mathcal{H}_{F_i^R}$.

Consider the following global intervention at $WX^{\rm out}Z^{\rm out}$. An agent is stationed at an additional locus E, such that for each node $N \in W$, the quantum system at $N^{\rm in}$ is sent to E, one half of a maximally entangled state is fed into $N^{\rm out}$, and the other half is sent to E. For each node $N \in Z$ or $N \in X$, one half of a maximally entangled state is fed into $N^{\rm out}$, and the other half is sent to E. This defines an operator $\sigma_{YZ^{\rm in}E}$ over Y, $Z^{\rm in}$ and E, with $\mathcal{H}_{E^{\rm in}}$ isomorphic to $\mathcal{H}_{W^{\rm in}} \otimes \mathcal{H}_{W^{\rm out}} \otimes \mathcal{H}_{X^{\rm out}} \otimes \mathcal{H}_{Z^{\rm out}}$, such that $\sigma_{YZ^{\rm in}E}$ has a block-diagonal structure with respect to the induced decomposition. Let $|i, f_i^L, f_i^R\rangle := J^{-1}\, |i, f_i^L\rangle\, |i, f_i^R\rangle$ label the induced orthonormal basis of $E^{\rm in}$ (for a suitable isomorphism J). The agent performs the von Neumann measurement at E corresponding to that basis. For a particular outcome k_E, corresponding to the basis state $|i, f_i^L, f_i^R\rangle$, define the operator

$$\begin{aligned}
&\mathrm{Tr}_E\Big[\sigma_{YZ^{\rm in}E}\ \ |i, f_i^L, f_i^R\rangle\, \langle i, f_i^L, f_i^R|\,\Big] \\
&\qquad = \ d_{E^{\rm out}}\ \ \langle i, f_i^L, f_i^R|\ \ J^{-1}\Big(\sum_j \alpha_{YF_j^L} \otimes \beta_{Z^{\rm in}F_j^R}\Big) J\ \ |i, f_i^L, f_i^R\rangle \\
&\qquad = \ d_{E^{\rm out}}\ \ \langle i, f_i^L|\, \alpha_{YF_i^L}\, |i, f_i^L\rangle\ \otimes\ \langle i, f_i^R|\, \beta_{Z^{\rm in}F_i^R}\, |i, f_i^R\rangle\ \ :=\ \gamma_Y \otimes \eta_{Z^{\rm in}}\ ,
\end{aligned}$$

where the $d_{E^{\rm out}}$ results from the trace over $E^{\rm out}$, on which σ_{YZE} acts trivially, and is then absorbed into, say γ_Y. The product form $\gamma_Y \otimes \eta_{Z^{\rm in}}$ implies that the joint probability distribution for k_E and outcomes k_Y and k_Z for an arbitrary intervention at Y, and an arbitrary local measurement of $Z^{\rm in}$, satisfies $P(k_Y, k_Z, k_E) = \phi(k_Y, k_E)\chi(k_Z, k_E)$ (for some functions ϕ and χ). Recalling Prop. 5.3, and noting that k_E is the outcome $k_{WX^{\rm out}Z^{\rm out}}$, this establishes the claim. □

A.13 Proof of Proposition 5.13

The proof is similar to that of Prop. 5.10.

(1) → (2):

Assume $\sigma_{YZW do(X)} = \alpha_{YWX^{\rm out}Z^{\rm out}}\beta_{ZWX^{\rm out}}$. As in the proof of Prop. 5.10, use the associativity and commutativity of the star-product, and express the operators in Condition (2) in terms of $\alpha^{\tau_Y}_{WX^{\rm out}Z^{\rm out}} := \mathrm{Tr}_Y\big[\tau_Y\ \alpha_{YWX^{\rm out}Z^{\rm out}}\big]$ and $\beta_{Z^{\rm out}WX^{\rm out}} := \mathrm{Tr}_{Z^{\rm in}}\big[\beta_{ZWX^{\rm out}}\big]$.

(2) → (3):

Consider the intervention at each node in Y that discards the input, and prepares a maximally mixed state on the output. Condition (2) then implies

$$\hat{\sigma}_{YZWdo(X)} \star \mathrm{Tr}_{YZ^{\mathrm{in}}}(\hat{\sigma}_{YZWdo(X)}) = \mathrm{Tr}_Y(\hat{\sigma}_{YZWdo(X)}) \star \mathrm{Tr}_{Z^{\mathrm{in}}}(\hat{\sigma}_{YZWdo(X)}),$$

which yields Condition (3).

(3) → (1):

The proof is the same as that of the proof of the (3) → (1) direction of Prop. 5.10, except that Z^{in} replaces Z, and $WX^{\mathrm{out}}Z^{\mathrm{out}}$ replaces WX^{out}. □

A.14 Proof of Thorem 5.7

Suppose $(Y \perp\!\!\!\perp Z|WX)_{G_{\overline{X}\underline{Z}}}$. Then Lemma A.2 implies $SR(Y, Z; WX)$ with respect to the mutilated DAG $G_{\overline{X}\underline{Z}}$. Hence, with the set X suppressed, there are partitions of the sets W and R such that allowed parent-child relationships are as shown in Fig. A.7.

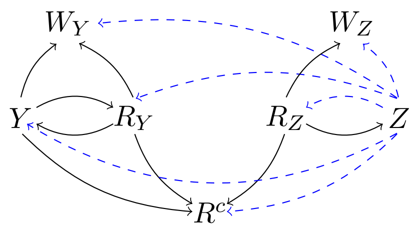


Figure A.7: The allowed parent-child relations in G, suppressing the set X, and suppressing arrows coming out of W_Y and W_Z. Blue dashed arrows represent parent-child relationships that are allowed in G, but absent in $G_{\overline{X}\underline{Z}}$.

Let σ_V be a process operator that is Markov for G. It follows from the above that, with a local intervention $\tau_R = \tau_{R_Y} \otimes \tau_{R_Z} \otimes \tau_{R^c}$ at the R nodes,

$$\begin{aligned} \sigma^{\tau_R}_{YZWdo(X)} \quad = \quad & \mathrm{Tr}_{R_Y}\left[\ \tau_{R_Y}\ \rho_{Y|Pa(Y)}\ \rho_{W_Y|Pa(W_Y)}\ \rho_{R_Y|Pa(R_Y)}\right] \\ & \mathrm{Tr}_{R_Z}\left[\ \tau_{R_Z}\ \rho_{Z|Pa(Z)}\ \rho_{W_Z|Pa(W_Z)}\ \rho_{R_Z|Pa(R_Z)}\ \right]\ , \end{aligned} \tag{A.29}$$

which is of the form $\sigma^{\tau_R}_{YZWdo(X)} = \alpha_{YWX^{\mathrm{out}}Z^{\mathrm{out}}}\ \beta_{ZWX^{\mathrm{out}}}$. □

A.15 Proof of Proposition 5.14

$(Y \perp\!\!\!\perp Set(Z)|Wdo(X))_{\kappa_{YZWX}} \Rightarrow$ (COS3):

Given a classical do-conditional process $\kappa_{YZWdo(X)}$, suppose that

$$\kappa^{\tau_Z}_{YWdo(X)} = \eta_{YWX^{\text{out}}}\ \xi^{\tau_Z}_{WX^{\text{out}}} \quad \forall \text{ local interventions } \tau_Z. \tag{A.30}$$

Consider an arbitrary local intervention at Y given by $P(k_Y, Y^{\text{out}}|Y^{\text{in}})$, a maximally informative local intervention at W given by

$$P(k_W, W^{\text{out}}|W^{\text{in}}) = \delta\big(g^{\text{in}}(k_W), W^{\text{in}}\big)\ \delta\big(g^{\text{out}}(k_W), W^{\text{out}}\big)\ P(k_W, W^{\text{out}}|W^{\text{in}}),$$

and a do-intervention at X that fixes $X^{\text{out}} = x$. For τ_Z a local intervention at Z, let $P^{\tau_Z}(k_Y, k_W)$ denote the resulting joint distribution over outcomes k_Y and k_W (where the notation suppresses dependence on x). This is given by

$$\begin{aligned} P^{\tau_Z}(k_Y, k_W) &= \sum_Y \sum_W \sum_{X^{\text{out}}} \kappa^{\tau_Z}_{YWdo(X)}\ P(k_Y, Y^{\text{out}}|Y^{\text{in}})\ \delta\big(X^{\text{out}}, x\big) \\ &\qquad \delta\big(g^{\text{in}}(k_W), W^{\text{in}}\big)\ \delta\big(g^{\text{out}}(k_W), W^{\text{out}}\big)\ P(k_W, W^{\text{out}}|W^{\text{in}}) \\ &= \sum_Y \eta_{YWX^{\text{out}}}(Y^{\text{in}}, Y^{\text{out}}, g^{\text{in}}(k_W), g^{\text{out}}(k_W), x)\ P(k_Y, Y^{\text{out}}|Y^{\text{in}}) \\ &\qquad \xi^{\tau_Z}_{WX^{\text{out}}}(g^{\text{in}}(k_W), g^{\text{out}}(k_W), x)\ P(k_W, g^{\text{out}}(k_W)|g^{\text{in}}(k_W))\ . \end{aligned}$$

Setting

$$\alpha(k_Y, k_W, x) = \sum_Y \eta_{YWX^{\text{out}}}(Y^{\text{in}}, Y^{\text{out}}, g^{\text{in}}(k_W), g^{\text{out}}(k_W), x)\ P(k_Y, Y^{\text{out}}|Y^{\text{in}}),$$

and

$$\beta^{\tau_Z}(k_W, x) = \xi^{\tau_Z}_{WX^{\text{out}}}(g^{\text{in}}(k_W), g^{\text{out}}(k_W), x)\ P(k_W, g^{\text{out}}(k_W)|g^{\text{in}}(k_W)),$$

yields $P^{\tau_Z}(k_Y, k_W) = \alpha(k_Y, k_W, x)\ \beta^{\tau_Z}(k_W, x)$, which implies that k_Y is independent of the choice of intervention τ_Z, conditioned on k_W. This holds for all interventions at Y, all maximally informative interventions at W, and all x, hence (COS3) follows.

(COS3) $\Rightarrow$ $(Y \perp\!\!\!\perp Set(Z)|W do(X))_{\kappa_{YZWX}}$:

Consider a classical process map κ_{YZWX}, and suppose that (COS3) holds for $\kappa_{YZWdo(X)}$. Consider local interventions at Y and W corresponding to an intervention at each node N ($N \in Y$ or $N \in W$) of the form

$$P(k_N, N^{\text{out}}|N^{\text{in}}) = \frac{1}{d_N}\delta(k^I_N, N^{\text{in}})\delta(k^O_N, N^{\text{out}}),$$

where d_N is the cardinality of the set on which N^{out} takes values. (Similar interventions were considered in Section A.6.) Let the joint outcome of the intervention at Y be $k_Y = (k_Y^I, k_Y^O)$, where k_Y^I is the tuple consisting of a value of k_N^I, for each $N \in Y$, and k_Y^O is the tuple consisting of a value of k_N^O, for each $N \in Y$. Similarly W and $k_W = (k_W^I, k_W^O)$. Consider a do-intervention at X that sets $X^{\text{out}} = x$, and an arbitrary local intervention τ_Z at Z.

As above, let $P^{\tau_Z}(k_Y, k_W)$ denote the resulting joint distribution over outcomes k_Y and k_W, given a local intervention τ_Z at Z, where the dependence on x is suppressed. The intervention at W is maximally informative, hence by assumption, the probability of outcome k_Y is independent of τ_Z when conditioned on k_W. This implies that there exist a function $\alpha(k_Y, k_W, x)$, and for each τ_Z, a function $\beta^{\tau_Z}(k_W, x)$, such that

$$P^{\tau_Z}(k_Y, k_W) = \alpha(k_Y, k_W, x)\ \beta^{\tau_Z}(k_W, x)\ . \tag{A.31}$$

Define $\eta_{YWX^{\text{out}}}$ such that

$$\eta_{YWX^{\text{out}}}(Y^{\text{in}}, Y^{\text{out}}, W^{\text{in}}, W^{\text{out}}, x) = d_Y d_W\ \alpha(k_Y, k_W, x)\big|_{k_Y=(Y^{\text{in}},Y^{\text{out}}),k_W=(W^{\text{in}},W^{\text{out}})}\ ,$$

and for each τ_Z, a function $\xi^{\tau_Z}_{WX^{\text{out}}}$ such that

$$\xi^{\tau_Z}_{WX^{\text{out}}}(W^{\text{in}}, W^{\text{out}}, x) = \beta^{\tau_Z}(k_W, x)\big|_{k_W=(W^{\text{in}},W^{\text{out}})}\ .$$

Observe that

$$\begin{aligned}
\alpha(k_Y, k_W, x) &= \sum_{YW} \eta_{YWX^{\text{out}}}\big|_{X^{\text{out}}=x} P(k_Y, Y^{\text{out}}|Y^{\text{in}}) P(k_W, W^{\text{out}}|W^{\text{in}})\ ,\\
\beta^{\tau_Z}(k_W, x) &= d_W \sum_{W} \xi^{\tau_Z}_{WX^{\text{out}}}\big|_{X^{\text{out}}=x}\ P(k_W, W^{\text{out}}|W^{\text{in}})\ .
\end{aligned}$$

Therefore,

$$\begin{aligned}
P^{\tau_Z}(k_Y, k_W) &= \alpha(k_Y, k_W, x)\ \beta^{\tau_Z}(k_W, x)\\
&= d_W\ \Big(\sum_{YW} \eta_{YWX^{\text{out}}}\big|_{X^{\text{out}}=x}\ P(k_Y, Y^{\text{out}}|Y^{\text{in}}) P(k_W, W^{\text{out}}|W^{\text{in}})\Big)\\
&\qquad \Big(\sum_{W} \xi^{\tau_Z}_{WX^{\text{out}}}\big|_{X^{\text{out}}=x}\ P(k_W, W^{\text{out}}|W^{\text{in}})\Big)\\
&= \sum_{YW} P(k_Y, Y^{\text{out}}|Y^{\text{in}})\ P(k_W, W^{\text{out}}|W^{\text{in}})\\
&\qquad \big(\eta_{YWX^{\text{out}}}\big)\big|_{X^{\text{out}}=x}\ \big(\xi^{\tau_Z}_{WX^{\text{out}}}\big)\big|_{X^{\text{out}}=x}\ .
\end{aligned} \tag{A.32}$$

From the definition of a classical process map,

$$P^{\tau_Z}(k_Y, k_W) = \sum_{YW} P(k_Y, Y^{\text{out}}|Y^{\text{in}})\ P(k_W, W^{\text{out}}|W^{\text{in}})\ \left(\kappa^{\tau_Z}_{YWdo(X)}\right)\big|_{X^{\text{out}}=x}. \quad \text{(A.33)}$$

The interventions considered at Y and W are informationally complete: that is, if for fixed k_Y, k_W, the term $P(k_Y, Y^{\text{out}}|Y^{\text{in}})P(k_W, W^{\text{out}}|W^{\text{in}})$ is viewed as a real-valued function of Y^{in}, Y^{out}, W^{in}, W^{out}, then, varying over k_Y, k_W, these functions span the vector space of all real-valued functions of Y^{in}, Y^{out}, W^{in}, W^{out}. Comparing Eqs. (A.32) and (A.33) then gives $\kappa^{\tau_Z}_{YZWdo(X)} = \eta_{YWX^{\text{out}}}\xi^{\tau_Z}_{WX^{\text{out}}}$, that is $(Y \perp\!\!\!\perp Set(Z)|Wdo(X))_{\kappa_{YZWX}}$. □

A.16 Proof of Proposition 5.15

This proof is again similar to that of Prop. 5.6.

Consider a process operator σ_{YZWX}, and assume that there is a Hermitian operator $\eta_{YWX^{\text{out}}}$, and for each local intervention τ_Z, a Hermitian operator $\xi^{\tau_Z}_{WX^{\text{out}}}$, such that

$$\sigma^{\tau_Z}_{YWdo(X)} = \eta_{YWX^{\text{out}}}\ \xi^{\tau_Z}_{WX^{\text{out}}}.$$

Note that $\eta_{YWX^{\text{out}}}$ commutes with $\xi^{\tau_Z}_{WX^{\text{out}}}$ for each τ_Z. The set $\{\xi^{\tau_Z}_{WX^{\text{out}}}\}$ for varying τ_Z generates a *-subalgebra of the form $\mathcal{A} = \mathbb{1}_Y \otimes \mathcal{A}_{WX^{\text{out}}}$, where $\mathcal{A}_{WX^{\text{out}}}$ is a *-subalgebra of $\mathcal{L}(\mathcal{H}_{W^{\text{in}}} \otimes \mathcal{H}^*_{W^{\text{out}}} \otimes \mathcal{H}^*_{X^{\text{out}}})$. A fundamental representation-theoretic result concerning finite-dimensional C*-algebras (see, e.g., Lemma 13 of Ref. [122]) then implies that there exists a decomposition $\mathcal{H}_{W^{\text{in}}} \otimes \mathcal{H}^*_{W^{\text{out}}} \otimes \mathcal{H}^*_{X^{\text{out}}} = \bigoplus_i \mathcal{H}_{F_i^L} \otimes \mathcal{H}_{F_i^R}$ such that $\mathcal{A}_{WX^{\text{out}}} = \bigoplus_i \mathbb{1}_{F_i^L} \otimes \mathcal{L}(\mathcal{H}_{F_i^R})$. The commutant $\mathcal{A}'$ of $\mathcal{A}$, that is, the subalgebra of operators that commute with all elements of $\mathcal{A}$, is of the form $\mathcal{A}' = \bigoplus_i \mathcal{L}(\mathcal{H}_Y \otimes \mathcal{H}_{F_i^L}) \otimes \mathbb{1}_{F_i^R}$. Since $\eta_{YWX^{\text{out}}} \in \mathcal{A}'$, and the distinct subspaces labelled by i are orthogonal, $\sigma^{\tau_Z}_{YWdo(X)}$ can be written in the form

$$\sigma^{\tau_Z}_{YWdo(X)} = \sum_i \eta_{YF_i^L} \otimes \xi^{\tau_Z}_{F_i^R}$$

for appropriate positive operators $\eta_{YF_i^L}$ and $\xi^{\tau_Z}_{F_i^R}$, where we have adopted the same convention as previously and let the latter operators act as zero maps on all other subspaces $j \neq i$. Consider a global intervention at WX^{out}, of the same form as that of (QOS1): that is, there is an additional locus E such that for each node $N \in W \cup X$, one half of a maximally entangled state is fed into N^{out}, and the other half sent to E, and for each node $N \in W$, the system at N^{in} is sent to E. The same arguments as in the proof of Prop. 5.6 imply that there exists a basis $\{|i, f_i^L, f_i^R\rangle\}$

of E^{in}, which corresponds to a basis $\{|i, f_i^L\rangle\, |i, f_i^R\rangle\}$ of $\bigoplus_i \mathcal{H}_{F_i^L} \otimes \mathcal{H}_{F_i^R}$. The agent at E performs the associated von Neumann measurement.

The probability of obtaining outcome k_Y for an arbitrary intervention $\tau_Y^{k_Y}$ at Y, and outcome k_E, corresponding to $|i, f_i^L, f_i^R\rangle$, for the von Neumann measurement at E, is

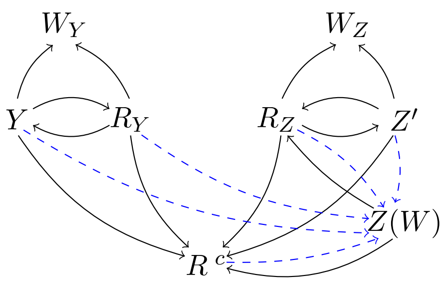
$$P(k_Y, k_E) = \mathrm{Tr}_Y\left[\langle i, f_i^L|\, \eta_{YF_i^L}\, |i, f_i^L\rangle\ \tau_Y^{k_Y}\right]\ \langle i, f_i^R|\, \xi_{F_i^R}^{\tau_Z}\, |i, f_i^R\rangle\ . \tag{A.34}$$

This product form implies that the probability of k_Y conditional on obtaining any of the outcomes at E is independent from τ_Z. □

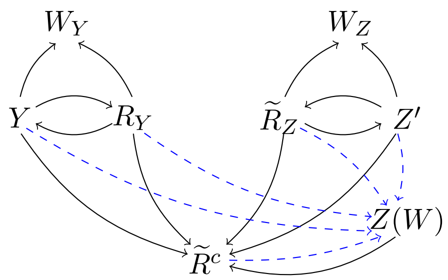
A.17 Proof of Theorem 5.9

Let G be a DAG with nodes $V = Y \cup Z \cup W \cup X \cup R$, for disjoint subsets Y, Z, W, X, and R, such that $(Y \perp\!\!\!\perp Z|WX)_{G_{\overline{XZ(W)}}}$. Then Lemma A.2 implies $SR(Y, Z; WX)$ with respect to the mutilated DAG $G_{\overline{XZ(W)}}$. There is therefore a partition of the set W into W_Y and W_Z, a partition of the set R into R_Y, R_Z and R^c, and a partition of the set Z into $Z(W)$ and $Z' = Z \backslash Z(W)$, such that, with X suppressed, the allowed parent-child relationships are as shown in Fig. A.8a. Note in particular that it follows from the definition of $Z(W)$ that there is no arrow from $Z(W)$ to W_Y, W_Z or Z'.

Let $\mathcal{R} := \{r \in R_Z : r \text{ is a descendant of a node in } Z(W)\}$ and define $\widetilde{R}_Z := R_Z \setminus \mathcal{R}$ and $\widetilde{R}^c := R^c \cup \mathcal{R}$. The allowed parent-child relationships between the resulting sets are shown in Fig. A.8b. Note in particular that there are no arrows from $\mathcal{R}$ to W_Y, W_Z or Z'.



(a) Allowed parent-child relations in G, with the set X, and arrows out of W_Y and W_Z suppressed. Blue dashed arrows show parent-child relationships that are allowed in G, but absent in $G_{\overline{XZ(W)}}$.



(b) Allowed parent-child relations in G, with re-defined sets $\widetilde{R}^c$ and $\widetilde{R}_Z$. The set X and arrows out of W_Y and W_Z are suppressed. Blue dashed arrows show parent-child relationships that are allowed in G, but absent in $G_{\overline{XZ(W)}}$.

Figure A.8

Let σ_V be a process operator that is Markov for G. The constraints on allowed parent-child relations shown in Fig. A.8b imply that for arbitrary local interventions $\tau_R = \tau_{R_Y} \otimes \tau_{\widetilde{R}_Z} \otimes \tau_{\widetilde{R}^c}$ and $\tau_Z = \tau_{Z(W)} \otimes \tau_{Z'}$,

$$\begin{aligned}
\sigma^{\tau_R,\tau_Z}_{YWdo(X)} \quad &= \quad \mathrm{Tr}_{Z'}\ \mathrm{Tr}_{R_Y}\ \mathrm{Tr}_{\widetilde{R}_Z}\Big[\tau_{Z'}\ \tau_{R_Y}\ \tau_{\widetilde{R}_Z}\ \rho_{Y|Pa(Y)}\ \rho_{W_Y|Pa(W_Y)}\ \rho_{R_Y|Pa(R_Y)} \\
&\qquad \rho_{Z'|Pa(Z')}\ \rho_{W_Z|Pa(W_Z)}\ \rho_{\widetilde{R}_Z|Pa(\widetilde{R}_Z)} \\
&\qquad \mathrm{Tr}_{\widetilde{R}^c}\ \mathrm{Tr}_{Z(W)}\big[\ \tau_{\widetilde{R}^c}\ \tau_{Z(W)}\ \rho_{Z(W)|Pa(Z(W))}\ \rho_{\widetilde{R}^c|Pa(\widetilde{R}^c)}\ \big]\ \Big] \\
&= \quad \mathrm{Tr}_{R_Y}\big[\ \tau_{R_Y}\ \rho_{Y|Pa(Y)}\ \rho_{W_Y|Pa(W_Y)}\ \rho_{R_Y|Pa(R_Y)}\ \big] \\
&\qquad \mathrm{Tr}_{Z'}\ \mathrm{Tr}_{\widetilde{R}_Z}\big[\ \tau_{Z'}\ \tau_{\widetilde{R}_Z}\ \rho_{Z'|Pa(Z')}\ \rho_{W_Z|Pa(W_Z)}\ \rho_{\widetilde{R}_Z|Pa(\widetilde{R}_Z)}\big]\ ,
\end{aligned}$$

where the second equality follows since

$$\mathrm{Tr}_{\widetilde{R}^c}\ \mathrm{Tr}_{Z(W)}\big[\ \tau_{\widetilde{R}^c}\ \tau_{Z(W)}\ \rho_{Z(W)|Pa(Z(W))}\ \rho_{\widetilde{R}^c|Pa(\widetilde{R}^c)}\ \big] = 1.$$

Setting

$$\eta_{YWX^{\mathrm{out}}} = \mathrm{Tr}_{R_Y}\big[\ \tau_{R_Y}\ \rho_{Y|Pa(Y)}\ \rho_{W_Y|Pa(W_Y)}\ \rho_{R_Y|Pa(R_Y)}\ \big],$$

and

$$\xi^{\tau_Z}_{WX^{\mathrm{out}}} = \mathrm{Tr}_{Z'}\ \mathrm{Tr}_{\widetilde{R}_Z}\big[\ \tau_{Z'}\ \tau_{\widetilde{R}_Z}\ \rho_{Z'|Pa(Z')}\ \rho_{W_Z|Pa(W_Z)}\ \rho_{\widetilde{R}_Z|Pa(\widetilde{R}_Z)}\big]$$

(where the notation suppresses the dependence of these quantities on τ_R), yields

$$\sigma^{\tau_R,\tau_Z}_{YWdo(X)} = \eta_{YWX^{\mathrm{out}}}\ \xi^{\tau_Z}_{WX^{\mathrm{out}}}.$$

Since the choices of τ_R and τ_Z were arbitrary, this gives that for all local interventions τ_R,

$$(Y \perp\!\!\!\perp Set(Z)|Wdo(X))_{\sigma^{\tau_R}_{YZWX}},$$

as required. □

Appendix B

Proofs and supplementary material Chapter 6

B.1 Proof of Lemma 6.2

Let $\rho_{Y|X}$ be a reduced unitary channel. By assumption there exists a Hilbert space $\mathcal{H}_F$, and a unitary transformation $U : \mathcal{H}_X \to \mathcal{H}_Y \otimes \mathcal{H}_F$, such that $\rho_{Y|X} = \mathrm{Tr}_F[\rho^U_{YF|X}]$.

In order to establish claim (1), suppose that $\rho_{Y|X} = \rho_{Y|X_1} \otimes \mathbb{1}_{X_2}$ with respect to some product structure $\mathcal{H}_X = \mathcal{H}_{X_1} \otimes \mathcal{H}_{X_2}$. Since $\rho_{Y|X_1} \otimes \mathbb{1}_{X_2} = \mathrm{Tr}_F[\rho^U_{YF|X_1X_2}]$, the unitary transformation U satisfies $X_2 \nrightarrow Y$. As shown in Section 6.2, this implies that there are unitary transformations $T : \mathcal{H}_{X_1} \to \mathcal{H}_Y \otimes \mathcal{H}_Z$ and $W : \mathcal{H}_Z \otimes \mathcal{H}_{X_2} \to \mathcal{H}_F$ such that $U = (\mathbb{1}_Y \otimes W)(T \otimes \mathbb{1}_{X_2})$. Hence $\rho_{Y|X_1} = \mathrm{Tr}_Z[\rho^T_{YZ|X_1}]$.

In order to establish claim (2), suppose that $\rho_{Y|X} = \bigoplus_i \rho_{Y|X_i}$ for some decomposition of $\mathcal{H}_X$ into orthogonal subspaces, $\mathcal{H}_X = \bigoplus_i \mathcal{H}_{X_i}$. By Theorem 4.1, the channel corresponding to the unitary transformation U can be written in the form $\rho^U_{YF|X} = \rho_{Y|X}\rho_{F|X}$. By Lemma 6.1, there exists a Hilbert space $\mathcal{H}_G = \bigoplus_j \mathcal{H}_{G^L_j} \otimes \mathcal{H}_{G^R_j}$, and a unitary transformation $V : \mathcal{H}_X \to \mathcal{H}_G$, with transpose $V^T : \mathcal{H}^*_G \to \mathcal{H}^*_X$, such that $\rho^U_{YF|X} = V^T \left(\bigoplus_j \rho_{Y|G^L_j} \otimes \rho_{F|G^R_j}\right) \left(V^T\right)^\dagger$. The fact that $\rho^U_{YF|X}$ is a rank 1 operator implies that this last equation cannot be satisfied if there is more than one term in the direct sum. Hence the index j takes only one value, and we can write $\mathcal{H}_G = \mathcal{H}_{G^L} \otimes \mathcal{H}_{G^R}$ such that $\rho^U_{YF|X} = V^T \left(\rho_{Y|G^L} \otimes \rho_{F|G^R}\right) \left(V^T\right)^\dagger$. Setting $\rho_{Y|G} := \rho_{Y|G^L} \otimes \mathbb{1}_{G^R}$, we have $\rho_{Y|X} = \sum_i \rho_{Y|X_i} = V^T \rho_{Y|G} \left(V^T\right)^\dagger$, where $\rho_{Y|X_i}$ is to be read as an operator on the whole of $\mathcal{H}_Y \otimes \mathcal{H}_X$, acting as zero map on all but the ith subspace $\mathcal{H}_Y \otimes \mathcal{H}_{X_i}$. Let $\rho_{Y|G_i} = \left(V^T\right)^\dagger \rho_{Y|X_i} V^T$, so that $\rho_{Y|G} = \sum_i \rho_{Y|G_i}$. Considering $(1/d_G)\rho_{Y|G}$ as a correctly normalised quantum state on $\mathcal{H}_Y \otimes \mathcal{H}_G$, the equation

$$\frac{1}{d_G}\rho_{Y|G} \;=\; \sum_i \frac{d_{G_i}}{d_G}\,\frac{1}{d_{G_i}}\rho_{Y|G_i} \;=\; \frac{1}{d_{G^L}}\rho_{Y|G^L}\otimes\frac{1}{d_{G^R}}\mathbb{1}_{G^R} \tag{B.1}$$

describes a convex decomposition of $(1/d_G)\rho_{Y|G}$, into states $(1/d_{G_i})\rho_{Y|G_i}$ with support on orthogonal subspaces. The fact that $(1/d_{G^L})\rho_{Y|G^L}$ is a pure, maximally entangled state implies that for each i,

$$\rho_{Y|G_i} \;=\; \rho_{Y|G^L}\otimes\phi^{(i)}_{G^R}\ , \tag{B.2}$$

for some appropriate operator $\phi^{(i)}_{G^R}$. Tracing Y on both sides of Eq. (B.2) yields

$$\mathbb{1}_{G^L}\otimes\phi^{(i)}_{G^R} \;=\; \mathbb{1}_{G_i}\ , \tag{B.3}$$

where on the right-hand side the zero maps on all but the ith subspace G_i are suppressed. Equation B.3 implies the existence of a subspace decomposition $\mathcal{H}_{G^R} = \bigoplus_i \mathcal{H}_{G^R_i}$ such that $\mathcal{H}_{G_i} = \mathcal{H}_{G^L}\otimes\mathcal{H}_{G^R_i}$ and $\phi^{(i)}_{G^R} = \mathbb{1}_{G^R_i}\oplus(\bigoplus_{j\neq i}0_{G^R_j})$. For each i, then, $\rho_{Y|G_i} = \rho_{Y|G^L}\otimes\mathbb{1}_{G^R_i}$. Let W be the unitary transformation corresponding to $\rho_{Y|G^L}$, and let $\widetilde{W} = W\otimes\mathbb{1}_{G^R_i}$. Then $\rho_{Y|G_i} = \mathrm{Tr}_{G^R_i}[\rho^{\widetilde{W}}_{YG^R_i|G^LG^R_i}]$, hence $\rho_{Y|G_i}$ represents a reduced unitary channel for each i, hence $\rho_{Y|X_i}$ represents a reduced unitary channel for each i. □

B.2 Proof of Theorem 6.4

Let $U:\mathcal{H}_{A_1}\otimes...\otimes\mathcal{H}_{A_n}\to\mathcal{H}_{B_1}\otimes...\otimes\mathcal{H}_{B_k}$ be a unitary transformation with causal structure $\{Pa^U(B_j)\}_{j=1}^k$. Let $j\in\{1,...,k\}$, and write $\overline{B_j} := \{B_1,...,B_k\}\setminus\{B_j\}$ and $\overline{Pa^U(B_j)} := \{A_1,...,A_n\}\setminus Pa^U(B_j)$. Regarding U as a bipartite unitary, with inputs $Pa^U(B_j)$, $\overline{Pa^U(B_j)}$, and outputs B_j, $\overline{B_j}$, such that $\overline{Pa^U(B_j)}\nrightarrow B_j$, the results of Section 6.2 imply the existence of $V:\mathcal{H}_{Pa^U(B_j)}\to\mathcal{H}_{B_j}\otimes\mathcal{H}_X$, and $W:\mathcal{H}_X\otimes\mathcal{H}_{\overline{Pa^U(B_j)}}\to\mathcal{H}_{\overline{B_j}}$, such that $U = (\mathbb{1}_{B_j}\otimes W)(V\otimes\mathbb{1}_{\overline{Pa^U(B_j)}})$. Hence $U^\dagger = (V^\dagger\otimes\mathbb{1}_{\overline{Pa^U(B_j)}})(\mathbb{1}_{B_j}\otimes W^\dagger)$, as illustrated in Fig. B.1.

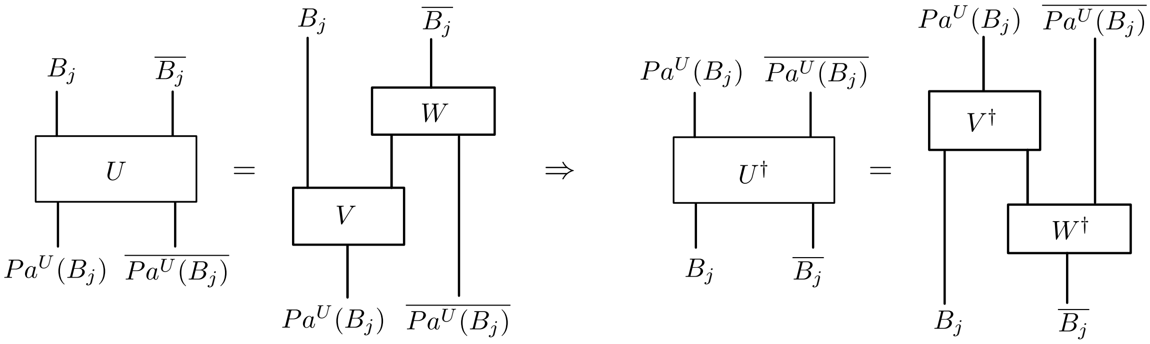


Figure B.1

It is thus manifest that $B_j \nrightarrow A_i$ in $U^\dagger$ for all $A_i \in \overline{Pa^U(B_j)}$. This is equivalent to the claim of Theorem 6.4.

□

B.3 Proof of Theorem 6.5

Let $U : \mathcal{H}_{A_1} \otimes \mathcal{H}_{A_2} \otimes \mathcal{H}_{A_3} \to \mathcal{H}_{B_1} \otimes \mathcal{H}_{B_2} \otimes \mathcal{H}_{B_3}$ be a unitary transformation. Suppose that the causal structure is as in Fig. 6.18a, i.e., $A_3 \nrightarrow B_1$, $A_2 \nrightarrow B_2$ and $A_1 \nrightarrow B_3$. Then, by Theorem 4.1, $\rho^U_{B_1B_2B_3|A_1A_2A_3} = \rho_{B_1|A_1A_2}\rho_{B_2|A_1A_3}\rho_{B_3|A_2A_3}$, where the factors on the right hand side commute pairwise. The commutation relation $[\rho_{B_1|A_1A_2}, \rho_{B_2|A_1A_3}] = 0$, along with Lemma 6.1, implies the existence of a unitary $S : \mathcal{H}_{A_1} \to \mathcal{H}_X = \bigoplus_i \mathcal{H}_{X_i^L} \otimes \mathcal{H}_{X_i^R}$ such that

$$\rho_{B_1|A_1A_2}\rho_{B_2|A_1A_3} = S^T \Big(\bigoplus_i \rho_{B_1|X_i^L A_2} \otimes \rho_{B_2|X_i^R A_3} \Big) \left(S^T\right)^\dagger , \tag{B.4}$$

for some appropriate families of channels $\{\rho_{B_1|X_i^L A_2}\}_i$ and $\{\rho_{B_2|X_i^R A_3}\}_i$. Hence

$$\rho^U_{B_1B_2B_3|A_1A_2A_3} = S^T \Big(\bigoplus_i \rho_{B_1|X_i^L A_2} \otimes \rho_{B_2|X_i^R A_3} \Big) \left(S^T\right)^\dagger \rho_{B_3|A_2A_3} . \tag{B.5}$$

Now, the operator $\rho_{B_3|A_2A_3}$ satisfies $S^T \rho_{B_3|A_2A_3} \left(S^T\right)^\dagger = \rho_{B_3|A_2A_3}$, where as always the necessary identity operators are suppressed in writing such products. Hence

$$\rho^U_{B_1B_2B_3|A_1A_2A_3} = S^T \Big(\bigoplus_i \rho_{B_1|X_i^L A_2} \otimes \rho_{B_2|X_i^R A_3} \Big) \rho_{B_3|A_2A_3} \left(S^T\right)^\dagger . \tag{B.6}$$

The operator $\rho_{B_3|A_2A_3}$ commutes with the factor in brackets to the left of it in Eq. B.6. Additionally, the operator $\rho_{B_3|A_2A_3}$ commutes with a projector onto the subspace $\mathcal{H}^*_{X_i} = \mathcal{H}^*_{X_i^L} \otimes \mathcal{H}^*_{X_i^R}$ of $\mathcal{H}^*_X$. This means that if $\rho_{B_1|X_i^L A_2} \otimes \rho_{B_2|X_i^R A_3}$ is regarded as an operator acting on the whole of $\mathcal{H}^*_X \otimes \mathcal{H}^*_{A_2} \otimes \mathcal{H}^*_{A_3} \otimes \mathcal{H}_{B_1} \otimes \mathcal{H}_{B_2}$, acting as the zero map on all but the ith subspace $\mathcal{H}^*_{X_i} \otimes \mathcal{H}^*_{A_2} \otimes \mathcal{H}^*_{A_3} \otimes \mathcal{H}_{B_1} \otimes \mathcal{H}_{B_2}$, then $\rho_{B_3|A_2A_3}$ commutes with $\rho_{B_1|X_i^L A_2} \otimes \rho_{B_2|X_i^R A_3}$ for each value of i. We can therefore write

$$\rho^U_{B_1B_2B_3|A_1A_2A_3} \;=\; S^T \left[\sum_i \left(\rho_{B_1|X_i^L A_2} \otimes \rho_{B_2|X_i^R A_3} \right) \rho_{B_3|A_2A_3} \right] \left(S^T\right)^\dagger \;, \tag{B.7}$$

where the ith term in the sum has non-trivial action only on the subspace $\mathcal{H}^*_{X_i} \otimes \mathcal{H}^*_{A_2} \otimes \mathcal{H}^*_{A_3} \otimes \mathcal{H}_{B_1} \otimes \mathcal{H}_{B_2} \otimes \mathcal{H}_{B_3}$. The fact that the left hand side of Eq. (B.7) is a rank 1 operator implies that there can only be one term in the sum, hence we can write $S : \mathcal{H}_{A_1} \rightarrow \mathcal{H}_{X^L} \otimes \mathcal{H}_{X^R}$ such that

$$\rho_{B_1|A_1A_2} \rho_{B_2|A_1A_3} = S^T \left(\rho_{B_1|X^L A_2} \otimes \rho_{B_2|X^R A_3} \right) \left(S^T\right)^\dagger . \tag{B.8}$$

Analogous arguments to that above yield unitaries $T : \mathcal{H}_{A_2} \rightarrow \mathcal{H}_{Y^L} \otimes \mathcal{H}_{Y^R}$ and $V : \mathcal{H}_{A_3} \rightarrow \mathcal{H}_{Z^L} \otimes \mathcal{H}_{Z^R}$, and corresponding channels, such that

$$\begin{aligned} \rho^U_{B_1B_2B_3|A_1A_2A_3} \;=\;& \left(S^T \otimes T^T \otimes V^T \right) \left(\rho_{B_1|X^L Y^L} \otimes \rho_{B_2|X^R Z^L} \otimes \rho_{B_3|Y^R Z^R} \right) \\ & \left(\left(S^T\right)^\dagger \otimes \left(T^T\right)^\dagger \otimes \left(V^T\right)^\dagger \right) . \end{aligned} \tag{B.9}$$

The product $\rho_{B_1|X^L Y^L} \otimes \rho_{B_2|X^R Z^L} \otimes \rho_{B_3|Y^R Z^R}$ represents a unitary channel, hence each factor individually represents a unitary channel. Denoting the respective unitary transformations $W : \mathcal{H}_{X^L} \otimes \mathcal{H}_{Y^L} \rightarrow \mathcal{H}_{B_1}$, $P : \mathcal{H}_{X^R} \otimes \mathcal{H}_{Z^L} \rightarrow \mathcal{H}_{B_2}$ and $Q : \mathcal{H}_{Y^R} \otimes \mathcal{H}_{Z^R} \rightarrow \mathcal{H}_{B_3}$, gives

$$U = (W \otimes P \otimes Q) \, (S \otimes T \otimes V) \;, \tag{B.10}$$

which concludes the proof. □

B.4 Proof of Theorem 6.6

Let $U : \mathcal{H}_{A_1} \otimes \mathcal{H}_{A_2} \otimes \mathcal{H}_{A_3} \rightarrow \mathcal{H}_{B_1} \otimes \mathcal{H}_{B_2} \otimes \mathcal{H}_{B_3} \otimes \mathcal{H}_{B_4}$ be a unitary transformation. Suppose that the causal structure of U is as in Fig. 6.21a, i.e., $A_3 \nrightarrow B_1$, $A_2 \nrightarrow B_2$ and $A_1 \nrightarrow B_3$. Then Theorem 4.1 implies that $\rho^U_{B_1B_2B_3B_4|A_1A_2A_3} = \rho_{B_1|A_1A_2} \; \rho_{B_2|A_1A_3} \; \rho_{B_3|A_2A_3} \; \rho_{B_4|A_1A_2A_3}$. Note that the causal structure is the same as in Fig. 6.18a of Theorem 6.5, apart from the additional output system B_4, which is influenced by all three input systems.

Considering the product $\rho_{B_1|A_1A_2} \; \rho_{B_2|A_1A_3} \; \rho_{B_3|A_2A_3}$, the same steps leading up to

Eq. (B.7) in the proof of Theorem 6.5 yield

$$\rho_{B_1B_2B_3|A_1A_2A_3} = S^T\left[\sum_i \left(\rho_{B_1|X_i^LA_2}\otimes\rho_{B_2|X_i^RA_3}\right)\rho_{B_3|A_2A_3}\right]\left(S^T\right)^\dagger , \tag{B.11}$$

for a unitary $S:\mathcal{H}_{A_1}\to\bigoplus_i\mathcal{H}_{X_i^L}\otimes\mathcal{H}_{X_i^R}$. This time, the term on the left hand side does not represent a unitary channel, hence we cannot conclude that there is only one term in the sum. The following analogous steps, leading up to Eq. (B.9) in the proof of Theorem 6.5 , then yield

$$\begin{aligned}\rho_{B_1B_2B_3|A_1A_2A_3} = & \left(S^T\otimes T^T\otimes V^T\right)\Big(\bigoplus_{i,j,k}\rho_{B_1|X_i^LY_j^L}\otimes\rho_{B_2|X_i^RZ_k^L}\otimes\rho_{B_3|Y_j^RZ_k^R}\Big)\\ & \Big(\left(S^T\right)^\dagger\otimes\left(T^T\right)^\dagger\otimes\left(V^T\right)^\dagger\Big) ,\end{aligned}$$

for unitaries $T:\mathcal{H}_{A_2}\to\bigoplus_j\mathcal{H}_{Y_j^L}\otimes\mathcal{H}_{Y_j^R}$ and $V:\mathcal{H}_{A_3}\to\bigoplus_k\mathcal{H}_{Z_k^L}\otimes\mathcal{H}_{Z_k^R}$.

By Lemma 6.2, each of the operators $\rho_{B_1|X_i^LY_j^L}$, $\rho_{B_2|X_i^RZ_k^L}$ and $\rho_{B_3|Y_j^RZ_k^R}$ represent reduced unitary channels for each i,j,k. Hence there exist families of unitaries of the form

$$P_{ij} : \mathcal{H}_{X_i^L}\otimes\mathcal{H}_{Y_j^L}\to\mathcal{H}_{B_1}\otimes\mathcal{H}_{F_{ij}^{(1)}} , \tag{B.12}$$

$$Q_{ik} : \mathcal{H}_{X_i^R}\otimes\mathcal{H}_{Z_k^L}\to\mathcal{H}_{B_2}\otimes\mathcal{H}_{F_{ik}^{(2)}} , \tag{B.13}$$

$$R_{jk} : \mathcal{H}_{Y_j^R}\otimes\mathcal{H}_{Z_k^R}\to\mathcal{H}_{B_3}\otimes\mathcal{H}_{F_{jk}^{(3)}} , \tag{B.14}$$

such that tracing $F_{ij}^{(1)}$, $F_{ik}^{(2)}$ and $F_{jk}^{(3)}$, respectively, for the induced unitary channels, gives back $\rho_{B_1|X_i^LY_j^L}$, $\rho_{B_2|X_i^RZ_k^L}$ and $\rho_{B_3|Y_j^RZ_k^R}$. Define $\mathcal{H}_F := \bigoplus_{i,j,k}\mathcal{H}_{F_{ij}^{(1)}}\otimes\mathcal{H}_{F_{ik}^{(2)}}\otimes\mathcal{H}_{F_{jk}^{(3)}}$ and the unitary $\widetilde{U}:\mathcal{H}_{A_1}\otimes\mathcal{H}_{A_2}\otimes\mathcal{H}_{A_3}\to\mathcal{H}_{B_1}\otimes\mathcal{H}_{B_2}\otimes\mathcal{H}_{B_3}\otimes\mathcal{H}_F$, by setting

$$\widetilde{U} := \Big(\bigoplus_{i,j,k}P_{ij}\otimes Q_{ik}\otimes R_{jk}\Big)\Big(S\otimes T\otimes V\Big) .$$

The unitary $\widetilde{U}$ is a unitary purification of the channel represented by $\rho_{B_1B_2B_3|A_1A_2A_3}$ and, by uniqueness of purification, can only differ from U by a unitary $W:\mathcal{H}_F\to\mathcal{H}_{B_4}$. This concludes the proof. □

B.5 Proof of Lemma 6.3

Let $\rho_{B_1B_2B_3|A_1A_2A_3A_4A_5} = \rho_{B_1|A_1A_3}\rho_{B_2|A_1A_2A_4}\rho_{B_3|A_1A_2A_5}$ be the CJ representation of a channel, where the factors on the right hand side commute pairwise. The commutation relation $[\rho_{B_1|A_1A_3}\ ,\ \rho_{B_2B_3|A_1A_2A_4A_5}] = 0$, where $\rho_{B_2B_3|A_1A_2A_4A_5} := \rho_{B_2|A_1A_2A_4}\ \rho_{B_3|A_1A_2A_5}$ yields, via Lemma 6.1, a decomposition

$$\rho_{B_1B_2B_3|A_1A_2A_3A_4A_5} = S^T \left(\bigoplus_i \rho_{B_1|X_i^L A_3} \otimes \rho_{B_2B_3|X_i^R A_2A_4A_5} \right) \left(S^T\right)^\dagger , \tag{B.15}$$

for some unitary $S : \mathcal{H}_{A_1} \to \mathcal{H}_X = \bigoplus_{i\in I} \mathcal{H}_{X_i^L} \otimes \mathcal{H}_{X_i^R}$. The marginal operators obtained by tracing B_1B_3, and B_1B_2, respectively define families of channels $\{\rho_{B_2|X_i^R A_2A_4}\}_i$ and $\{\rho_{B_3|X_i^R A_2A_5}\}_i$. The commutation relation $[\rho_{B_2|A_1A_2A_4}, \rho_{B_3|A_1A_2A_5}] = 0$ implies $[\rho_{B_2|XA_2A_4}, \rho_{B_3|XA_2A_5}] = 0$, where $\rho_{B_2|XA_2A_4} = \bigoplus_i \mathbb{1}_{(X_i^L)^*} \otimes \rho_{B_2|X_i^R A_2A_4}$ and $\rho_{B_3|XA_2A_5} = \bigoplus_i \mathbb{1}_{(X_i^L)^*} \otimes \rho_{B_3|X_i^R A_2A_5}$. The fact that each of $\rho_{B_2|XA_2A_4}$ and $\rho_{B_3|XA_2A_5}$ commutes with a projector onto $\mathcal{H}^*_{X_i} := \mathcal{H}^*_{X_i^L} \otimes \mathcal{H}^*_{X_i^R}$ implies that $[\rho_{B_2|X_i^R A_2A_4}\ ,\ \rho_{B_3|X_i^R A_2A_5}] = 0$ for each i. Thus, iterating the argument, there exists for each i a unitary $T_i : \mathcal{H}_{X_i^R} \otimes \mathcal{H}_{A_2} \to \bigoplus_{j_i\in J_i} \mathcal{H}_{Y_{ij_i}^L} \otimes \mathcal{H}_{Y_{ij_i}^R}$ with $\{J_i\}$ a family of sets parametrized by $i \in I$, such that Eq. (6.6) holds. □

B.6 Proof of Theorem 6.7

Let $U : \mathcal{H}_{A_1} \otimes \mathcal{H}_{A_2} \otimes \mathcal{H}_{A_3} \otimes \mathcal{H}_{A_4} \to \mathcal{H}_{B_1} \otimes \mathcal{H}_{B_2} \otimes \mathcal{H}_{B_3} \otimes \mathcal{H}_{B_4}$ be a unitary transformation. Suppose that the causal structure is as in Fig. 6.38a, i.e., $A_4 \nrightarrow B_1$, $A_2 \nrightarrow B_2$, $A_4 \nrightarrow B_2$, $A_1 \nrightarrow B_3$, and $A_2 \nrightarrow B_3$. Then Theorem 4.1 implies that $\rho^U_{B_1B_2B_3B_4|A_1A_2A_3A_4} = \rho_{B_1|A_1A_2A_3}\ \rho_{B_2|A_1A_3}\ \rho_{B_3|A_3A_4}\ \rho_{B_4|A_1A_2A_3A_4}$. The proof proceeds analogously to that of Theorem 6.6, only that this time there will be a 'nested splitting'. Due to Lemma 6.3, the pairwise commutation relations between $\rho_{B_1|A_1A_2A_3}$, $\rho_{B_2|A_1A_3}$ and $\rho_{B_3|A_3A_4}$ yield a unitary $S : \mathcal{H}_{A_3} \to \bigoplus_i \mathcal{H}_{X_i^L} \otimes \mathcal{H}_{X_i^R}$ and for each i a unitary $T_i : \mathcal{H}_{A_1} \otimes \mathcal{H}_{X_i^L} \to \bigoplus_{j_i} \mathcal{H}_{Y_{ij_i}^L} \otimes \mathcal{H}_{Y_{ij_i}^R}$ such that

$$\begin{aligned} \rho_{B_1B_2B_3|A_1A_2A_3A_4} &= \\ & S^T \left[\bigoplus_i \left(T_i^T \Big(\bigoplus_{j_i} \rho_{B_1|A_2Y_{ij_i}^L} \otimes \rho_{B_2|Y_{ij_i}^R} \Big) \left(T_i^T\right)^\dagger \right) \otimes \rho_{B_3|X_i^R A_4} \right] \left(S^T\right)^\dagger . \end{aligned}$$

Due to Lemma 6.2, the operators $\rho_{B_1|A_2Y_{ij_i}^L}$, $\rho_{B_2|Y_{ij_i}^R}$ and $\rho_{B_3|X_i^R A_4}$ represent reduced unitary channels for each i, j_i. Hence there exist families of unitary transformations of the form

$$\begin{aligned} P_{ij_i} &: \mathcal{H}_{A_2} \otimes \mathcal{H}_{Y_{ij_i}^L} \to \mathcal{H}_{B_1} \otimes \mathcal{H}_{F_{ij_i}^L} , \\ Q_{ij_i} &: \mathcal{H}_{Y_{ij_i}^R} \to \mathcal{H}_{B_2} \otimes \mathcal{H}_{F_{ij_i}^R} , \\ V_i &: \mathcal{H}_{X_i^R} \otimes \mathcal{H}_{A_4} \to \mathcal{H}_{G_i^R} \otimes \mathcal{H}_{B_3} , \end{aligned}$$

such that tracing $F^L_{ij_i}$, $F^R_{ij_i}$ and G^R_i, respectively, for the induced unitary channels, gives back $\rho_{B_1|A_2Y^L_{ij_i}}$, $\rho_{B_2|Y^R_{ij_i}}$ and $\rho_{B_3|X^R_iA_4}$. For each i, let T'_i be a unitary transformation $T'_i : \bigoplus_{j_i} \mathcal{H}_{F^L_{ij_i}} \otimes \mathcal{H}_{F^R_{ij_i}} \to \mathcal{H}_{G^L_i}$, for some Hilbert space $\mathcal{H}_{G^L_i}$. Define $\mathcal{H}_G := \bigoplus_i \mathcal{H}_{G^L_i} \otimes \mathcal{H}_{G^R_i}$. By construction, the following unitary transformation $\widetilde{U} : \mathcal{H}_{A_1} \otimes \mathcal{H}_{A_2} \otimes \mathcal{H}_{A_3} \otimes \mathcal{H}_{A_4} \to \mathcal{H}_{B_1} \otimes \mathcal{H}_{B_2} \otimes \mathcal{H}_{B_3} \otimes \mathcal{H}_G$ constitutes a unitary purification of the channel represented by $\rho_{B_1B_2B_3|A_1A_2A_3A_4}$:

$$\widetilde{U} := \Big[\bigoplus_i \Big(\mathbb{1}_{B_1} \otimes T'_i \otimes \mathbb{1}_{B_2}\Big)\Big(\bigoplus_{j_i} P_{ij_i} \otimes Q_{ij_i}\Big)\Big(\mathbb{1}_{A_2} \otimes T_i\Big) \ \otimes V_i\Big]\Big(\mathbb{1}_{A_1A_2} \otimes S \otimes \mathbb{1}_{A_4}\Big).$$

By uniqueness of purification, $\widetilde{U}$ can differ from U only by a unitary transformation $S' : \mathcal{H}_G \to \mathcal{H}_{B_4}$, which concludes the proof. □

B.7 Proof of Theorem 6.8

Let $U : \mathcal{H}_{A_1} \otimes \mathcal{H}_{A_2} \otimes \mathcal{H}_{A_3} \otimes \mathcal{H}_{A_4} \to \mathcal{H}_{B_1} \otimes \mathcal{H}_{B_2} \otimes \mathcal{H}_{B_3} \otimes \mathcal{H}_{B_4}$ be a unitary transformation. Suppose that the causal structure is as in Fig. 6.39a. This is the same causal structure as in Fig. 6.21a of Theorem 6.6 with the only difference that B_3 and B_4 now have one additional parent, A_4. It is straightforward to follow the same steps as in the proof of Theorem 6.6 since they are not affected by the additional non-trivial action of $\rho_{B_3|A_2A_3A_4}$ on A_4. The claim is then immediate. □

B.8 Proof Theorem 6.9

Let $U : \mathcal{H}_{A_1} \otimes \mathcal{H}_{A_2} \otimes \mathcal{H}_{A_3} \otimes \mathcal{H}_{A_4} \to \mathcal{H}_{B_1} \otimes \mathcal{H}_{B_2} \otimes \mathcal{H}_{B_3} \otimes \mathcal{H}_{B_4}$ be a unitary transformation. Suppose that the causal structure is as in Fig. 6.40a, i.e., $A_3 \nrightarrow B_1$, $A_4 \nrightarrow B_1$, $A_2 \nrightarrow B_2$, $A_4 \nrightarrow B_2$, $A_1 \nrightarrow B_3$ and $A_2 \nrightarrow B_3$. Then Theorem 4.1 implies that $\rho^U_{B_1B_2B_3B_4|A_1A_2A_3A_4} = \rho_{B_1|A_1A_2}\ \rho_{B_2|A_1A_3}\ \rho_{B_3|A_3A_4}\ \rho_{B_4|A_1A_2A_3A_4}$. The rest of the proof is analogous to that of Theorem 6.6, and will not be stated in full detail. The commutation relations $[\rho_{B_1|A_1A_2}, \rho_{B_2|A_1A_3}] = 0$ and $[\rho_{B_2|A_1A_3}, \rho_{B_3|A_3A_4}] = 0$ give independent decompositions of A_1 and A_3, captured by the unitaries S and T as depicted in Fig. 6.40b. Lemma 6.2 and uniqueness of purification then yield the claim that

$$U = \Big(\mathbb{1}_{B_1B_2B_3} \otimes V\Big)\Big(\bigoplus_{i,j} P_i \otimes Q_{ij} \otimes R_j\Big)\Big(S \otimes \mathbb{1}_{A_2} \otimes T \otimes \mathbb{1}_{A_4}\Big)\,. \qquad \square$$

B.9 Proof Theorem 6.10

Let $U : \mathcal{H}_{A_1} \otimes \mathcal{H}_{A_2} \otimes \mathcal{H}_{A_3} \otimes \mathcal{H}_{A_4} \to \mathcal{H}_{B_1} \otimes \mathcal{H}_{B_2} \otimes \mathcal{H}_{B_3} \otimes \mathcal{H}_{B_4}$ be a unitary transformation. Suppose that the causal structure is as in Fig. 6.41a, i.e., $A_3 \nrightarrow B_2$, $A_4 \nrightarrow B_2$, $A_2 \nrightarrow B_3$, $A_4 \nrightarrow B_3$, $A_2 \nrightarrow B_4$ and $A_3 \nrightarrow B_4$. Then Theorem 4.1 implies that $\rho^U_{B_1B_2B_3B_4|A_1A_2A_3A_4} = \rho_{B_1|A_1A_2A_3A_4}\ \rho_{B_2|A_1A_2}\ \rho_{B_3|A_1A_3}\ \rho_{B_4|A_1A_4}$. Given the pairwise commutation relations between the operators $\rho_{B_2|A_1A_2}$, $\rho_{B_3|A_1A_3}$ and $\rho_{B_4|A_1A_4}$, an iterative application of Lemma 6.1, analogously to the proof of Lemma 6.3, together with the fact that the only Hilbert space on which the respective non-trivial actions of the three operators overlap is $\mathcal{H}_{A_1}$, implies that there exists a unitary $S : \mathcal{H}_{A_1} \to \bigoplus_i \mathcal{H}_{X_i^{(1)}} \otimes \mathcal{H}_{X_i^{(2)}} \otimes \mathcal{H}_{X_i^{(3)}}$ such that

$$\rho_{B_2|A_1A_2}\ \rho_{B_3|A_1A_3}\ \rho_{B_4|A_1A_4} = S^T \left(\bigoplus_i \rho_{B_2|X_i^{(1)}A_2} \otimes \rho_{B_3|X_i^{(2)}A_3} \otimes \rho_{B_4|X_i^{(3)}A_4} \right) \left(S^T\right)^\dagger .$$

The rest of the proof proceeds by analogous arguments as the proof of Thm. 6.6, that is, due to Lemma 6.2 there exist families of unitaries $P_i : \mathcal{H}_{X_i^{(1)}} \otimes \mathcal{H}_{A_2} \to \mathcal{H}_{Y_i^{(1)}} \otimes \mathcal{H}_{B_2}$, $Q_i : \mathcal{H}_{X_i^{(2)}} \otimes \mathcal{H}_{A_3} \to \mathcal{H}_{Y_i^{(2)}} \otimes \mathcal{H}_{B_3}$ and $R_i : \mathcal{H}_{X_i^{(3)}} \otimes \mathcal{H}_{A_4} \to \mathcal{H}_{Y_i^{(3)}} \otimes \mathcal{H}_{B_4}$ and furthermore, by uniqueness of purification, a unitary $T : \bigoplus_i \mathcal{H}_{Y_i^{(1)}} \otimes \mathcal{H}_{Y_i^{(2)}} \otimes \mathcal{H}_{Y_i^{(3)}} \to \mathcal{H}_{B_1}$ such that

$$U = \left(T \otimes \mathbb{1}_{B_2B_3B_4}\right)\left(\bigoplus_i P_i \otimes Q_i \otimes R_i\right)\left(S \otimes \mathbb{1}_{A_2A_3A_4}\right) .$$

□

Appendix C

Proofs and supplementary material Chapter 7

C.1 Characterisation of process operators

Let $\{\eta_X^l\}_{l=0}^{d_X^2-1}$ denote a Hilbert-Schmidt (HS) basis for $\mathcal{L}(\mathcal{H}_X)$, i.e., a set of operators such that they are orthonormal with respect to the HS inner product and, in addition, traceless for all $l = 1, ..., d_X^2 - 1$, while $\eta_X^0 = (1/d_X)\mathbb{1}_X$. Any $\sigma \in \mathcal{L}(\mathcal{H}_{A^{\text{in}}} \otimes \mathcal{H}^*_{A^{\text{out}}} \otimes \mathcal{H}_{B^{\text{in}}} \otimes \mathcal{H}^*_{B^{\text{out}}})$ can be expanded in a HS basis as $\sigma = \sum_{l_1,l_2,l_3,l_4} \alpha_{l_1 l_2 l_3 l_4} \eta^{l_1}_{A^{\text{in}}} \otimes \eta^{l_2}_{A^{\text{out}}} \otimes \eta^{l_3}_{B^{\text{in}}} \otimes \eta^{l_4}_{B^{\text{out}}}$. A term of type A^{in} in the expansion is a summand with non-trivial action only on A^{in}, i.e. $l_1 \neq 0$ and $l_2 = l_3 = l_4 = 0$. Similarly for types $A^{\text{in}}B^{\text{out}}$ etc.

It was shown in Ref. [43] that σ being a bipartite process operator is equivalent to $\sigma \geq 0$, $\text{Tr}[\sigma] = d_{A^{\text{out}}} d_{B^{\text{out}}}$ and that in a HS basis expansion, in addition to a term, which is proportional to the identity operator on all four spaces, only the coefficients of terms of the types A^{in}, B^{in}, $A^{\text{in}}B^{\text{in}}$, $A^{\text{in}}B^{\text{out}}$, $A^{\text{out}}B^{\text{in}}$, $A^{\text{in}}A^{\text{out}}B^{\text{in}}$ and $A^{\text{in}}B^{\text{in}}B^{\text{out}}$, may be non-vanishing. These conditions were generalized to n numbers of parties in Ref. [49] and can easily be stated as (1) $\sigma \geq 0$, (2) $\text{Tr}[\sigma] = \prod_{i=1}^n d_{A_i^{\text{out}}}$ and (3) that in a HS basis expansion the only non-vanishing terms, apart from an overall identity operator, are of a type such that there must be at least one node, say A_i, on whose out-space, A_i^{out}, the action is trivial, but on whose in-space, A_i^{in}, the action is non-trivial. Equivalent conditions were presented in [48] where the projector onto the linear subspace of process operators was defined explicitly, giving a basis-independent characterization.

C.2 Proof of Proposition 7.1

Suppose (G, σ_{AB}) is a cyclic QCM with G as in Fig. 7.1a. By Markovianity for G, it holds that $\sigma_{AB} = \rho_{A|B}\ \rho_{B|A}$, which due to our convention reads $\sigma_{AB} = \rho_{B|A} \otimes \rho_{A|B}$, as both factors act on distinct Hilbert spaces. Further suppose that this is a faithful QCM, i.e., both channels $\rho_{A|B}$ and $\rho_{B|A}$ are signalling channels. One way to see that this contradicts the assumption that σ_{AB} is a valid process is by analyzing the non-vanishing types of terms in an expansion of σ_{AB} relative to a Hilbert-Schmidt product basis (see Sec. C.1). If signalling from B^{out} to A^{in} is possible through $\rho_{A|B}$, then an expansion of just $\rho_{A|B}$ has to contain a non-vanishing term of type $A^{\text{in}}B^{\text{out}}$. Similarly, if signalling from A^{out} to B^{in} is possible in $\rho_{B|A}$, then an expansion of $\rho_{B|A}$ has to contain a non-vanishing term of type $B^{\text{in}}A^{\text{out}}$. Consequently, σ_{AB} has to contain a non-vanishing term of type $A^{\text{in}}B^{\text{out}}B^{\text{in}}A^{\text{out}}$, which is forbidden for a process operator [43].

C.3 Commutation insufficient for being a process operator

Sec. 7.2.2 observed that not every cyclic directed graph is the causal structure of some faithful QCM (established, e.g., by Prop. 7.1). It furthermore claimed that even given a cyclic directed graph G that does accommodate a faithful QCM, it is not true that then any product of commuting operators $\prod_i \rho_{A_i|Pa(A_i)}$, with parental sets as in G, defines a process operator. The following gives a simple example to back this claim.

Consider the cyclic graph G with three vertices A, B and C from Fig. 7.1b. As observed in Sec. 7.4.1 G is the causal structure of a faithful QCM. Let A, B and C be classical split nodes (see Sec. 7.6), where all input and output variables A^{in}, A^{out}, B^{in}, B^{out}, C^{in} and C^{out} are classical bits. Let furthermore classical channels be given as in Eqs. C.1-C.2. One can easily check that the dependencies in $P(A^{\text{in}}|B^{\text{out}}, C^{\text{out}})$ and $P(B^{\text{in}}|A^{\text{out}}, C^{\text{out}})$ are such that Fig. 7.1b indeed represents the signalling relations. However, note that for any probability distribution $P(C^{\text{in}})$, the product $P(A^{\text{in}}|B^{\text{out}}, C^{\text{out}})P(B^{\text{in}}|A^{\text{out}}, C^{\text{out}})P(C^{\text{in}})$ is not a classical process. This can be seen from considering a do-intervention at C that fixes $C^{\text{out}} = 0$, since the classical channels $P(A^{\text{in}}|B^{\text{out}}, 0)$ and $P(B^{\text{in}}|A^{\text{out}}, 0)$ are still signalling and seeing them as special cases of quantum channels gives a contradiction with Prop. 7.1.

$$P(A^{\text{in}}|B^{\text{out}}, C^{\text{out}}) := \begin{cases} P(0|0,0) = 0.4, & P(0|0,1) = 0.3, \\ P(1|0,0) = 0.6, & P(1|0,1) = 0.7, \\ P(0|1,0) = 0.8, & P(0|1,1) = 0.3, \\ P(1|1,0) = 0.2, & P(1|1,1) = 0.7. \end{cases} \tag{C.1}$$

$$P(B^{\text{in}}|A^{\text{out}}, C^{\text{out}}) := \begin{cases} P(0|0,0) = 0.5, & P(0|0,1) = 0.3, \\ P(1|0,0) = 0.5, & P(1|0,1) = 0.7, \\ P(0|1,0) = 0.25, & P(0|1,1) = 0.1, \\ P(1|1,0) = 0.75, & P(1|1,1) = 0.9. \end{cases} \tag{C.2}$$

C.4 Definition causal separability

Section 7.1.1 mentioned the notion of causal separability, however, it only gave a precise definition for the bipartite case. As already mentioned there, in the general multipartite case the definition is a little more intricate, because arguably it should include cases where the causal order of a subset of nodes may depend on the operation at an earlier node, as well as it should be such that a process remains causally separable even if extending the process with additional input states shared among all nodes. The below definition was given in Ref. [64] and therein shown to be equivalent to an earlier version presented in Ref. [49]. It is an iterative definition, which relies on the notion of no-signalling between the nodes of a quantum process from Def. 3.8. In order to avoid clutter, we here write τ_{A_j}, in slight abuse of notation, for the representation of a CP map at the node A_j, also if it is not trace-preserving. While given a quantum process $\sigma_{A_1 \ldots A_n}$, the object $\text{Tr}_{A_j}[\sigma_{A_1 \ldots A_n} \tau_{A_j}]$ is not generally a process operator, if A_j cannot signal to $\{A_1, \ldots, A_n\} \setminus \{A_j\}$, then it is proportional to a process operator. In the latter case we refer to the corresponding correctly normalized process operator as the *conditional process* and denote it as $\sigma|_{\tau_{A_j}}$.

Definition C.1 (Causal separability) [64]: *Every single-node process is* causally separable. *For $n \geq 2$, a process σ on n quantum nodes A_1, ..., A_n is said to be* causally separable*, if and only if, for any extension of each node A_j with an additional input system $\mathcal{H}_{(A'_j)^{in}}$ to a new node $\widetilde{A}_j$, defined by $\mathcal{H}_{\widetilde{A}_j^{in}} := \mathcal{H}_{A_j^{in}} \otimes \mathcal{H}_{(A'_j)^{in}}$ and $\mathcal{H}_{\widetilde{A}_j^{out}} := \mathcal{H}_{A_j^{out}}$, and any auxiliary quantum state $\rho \in \mathcal{L}(\mathcal{H}_{(A'_1)^{in}} \otimes \ldots \otimes \mathcal{H}_{(A'_n)^{in}})$,* *the process $\sigma \otimes \rho$ on the quantum nodes $\widetilde{A}_1, \ldots, \widetilde{A}_n$ decomposes as*

$$\sigma \otimes \rho \;=\; \sum_{k=1}^{n} q_k \; \sigma^{\rho}_{(k)}, \tag{C.3}$$

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

C.5 Proof of Theorem 7.4

First, suppose $\kappa_{X_1 \ldots X_n}$ is a reversibly extendible process, that is, there exists a reversible deterministic process $\kappa^{g}_{X_1 \ldots X_n \lambda F}$ for some bijection $g : X_1^{\text{out}} \times \ldots \times X_n^{\text{out}} \times \lambda^{\text{out}} \to X_1^{\text{in}} \times \ldots \times X_n^{\text{in}} \times F^{\text{in}}$, such that

$$\kappa_{X_1 \ldots X_n} = \sum_{\lambda^{\text{out}}, F^{\text{in}}} \kappa^{g}_{X_1 \ldots X_n \lambda F} \; P(\lambda^{\text{out}}) \tag{C.4}$$

for some probability distribution $P(\lambda^{\text{out}})$. It follows from the fact that $\kappa^{g}_{X_1 \ldots X_n \lambda F}$ is a classical process that marginalization as in Eq. C.4 has to yield a classical process over nodes $X_1, \ldots, X_n$ for arbitrary distributions $P(\lambda^{\text{out}})$, in particular for every point-distribution. Hence, for every value λ' of λ^{out}, the induced function $g_{\lambda'}(\_\_) := g(\_\_, \lambda')$ has to define a deterministic process for $n+1$ nodes and furthermore, also once marginalizing over F it still has to be a deterministic process for the n nodes $X_1, \ldots, X_n$. Hence, Eq. C.4 can be read as establishing that the given $\kappa_{X_1 \ldots X_n}$ is a convex mixture of deterministic processes over the nodes $X_1, \ldots, X_n$, i.e. $\kappa_{X_1 \ldots X_n}$ lies in the deterministic polytope.

Conversely, suppose $\kappa_{X_1 \ldots X_n}$ lies inside the deterministic polytope, that is, there exists a family of deterministic processes $\{\kappa^{f_i}_{X_1 \ldots X_n}\}_{i=1}^{m}$, defined by the functions $f_i : X_1^{\text{out}} \times \ldots \times X_n^{\text{out}} \to X_1^{\text{in}} \times \ldots \times X_n^{\text{in}}$ such that $\kappa_{X_1 \ldots X_n} = \sum_{i=1}^{m} q_i \; \kappa^{f_i}_{X_1 \ldots X_n}$ for some probability distribution $\{q_i\}$. The proof will proceed by first observing that such a process can be seen to arise from one single deterministic process on $n+2$ nodes. Together with the fact that every deterministic process is reversibly extendible, proven in Ref. [58], this establishes the claim. In order to see that indeed an appropriate deterministic process on $n+2$ nodes exists, let λ^{out} and F^{in} be variables with cardinality m and define the function

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

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

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